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Title: A Multiscale, Conservative, Implicit 1D-2V Multispecies Vlasov-Fokker-Planck Solver for ICF Capsule Implosion Simulations

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A Multiscale, Conservative, Implicit 1D-2V Multispecies Vlasov-Fokker-Planck Solver for ICF Capsule Implosion Simulations

CCAM Seminar, Purdue U.

Feb. 12th, 2018

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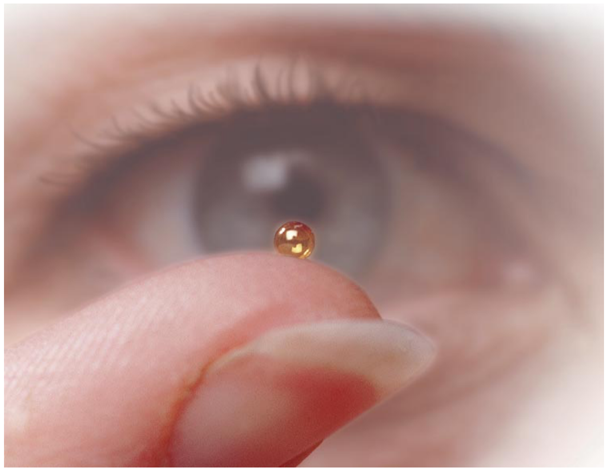
Agenda

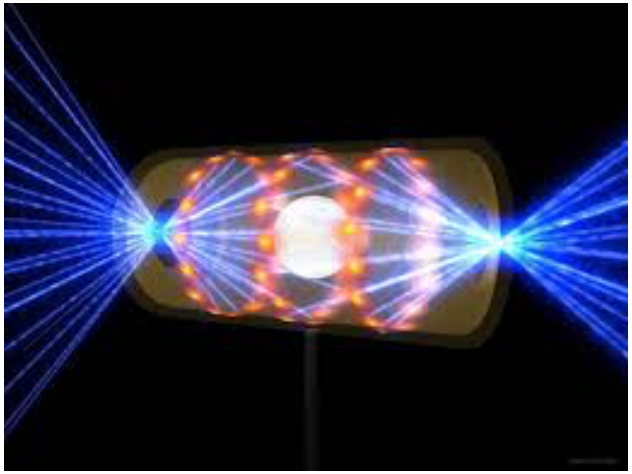
Feb. 12, 2018

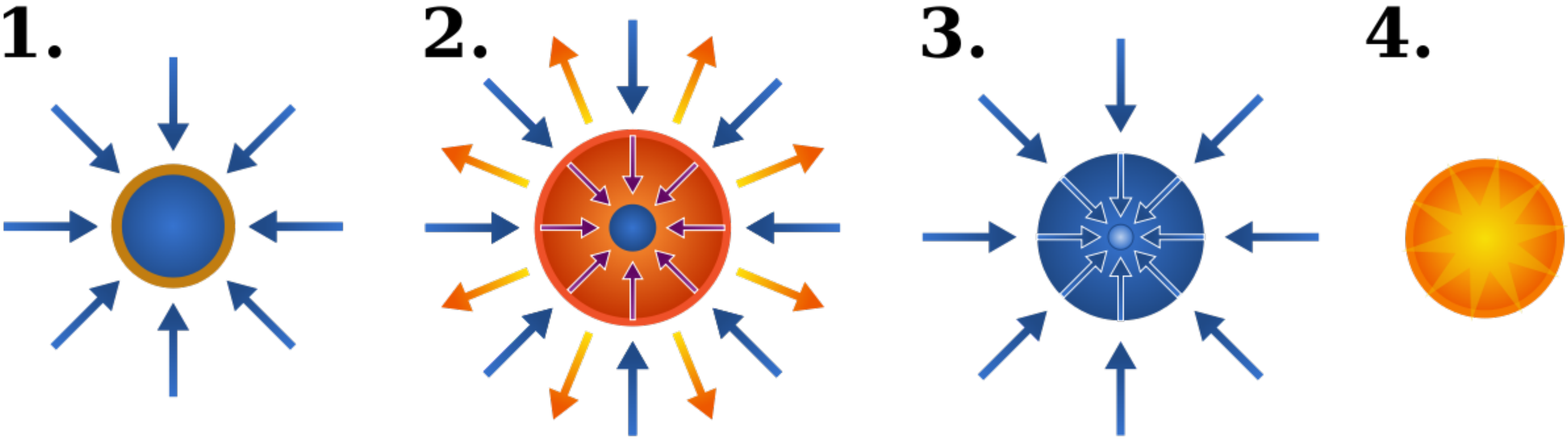
CCAM Seminar, Purdue U.

- Motivation and challenges of Rosenbluth-VFP
  - Moderate Knudsen numbers are common in ICF implosions
  - Temporal and spatial resolution requirements
- What we bring to the table
  - Multi-species Vlasov-Rosenbluth-Fokker-Planck + fluid electrons + radiation (eventually)
  - Asymptotic well posedness
    - Fully implicit, nonlinear formulation
    - Fully conservative discrete implementation (mass, momentum, and energy)
  - Orders of magnitude algorithmic speedups
    - Fully implicit timestepping [O(N)]
    - Velocity space dynamic adaptivity
    - Asymptotic treatment of collision operator for disparate v_{th} ratios
- Numerical verification and application of the algorithm to ICF

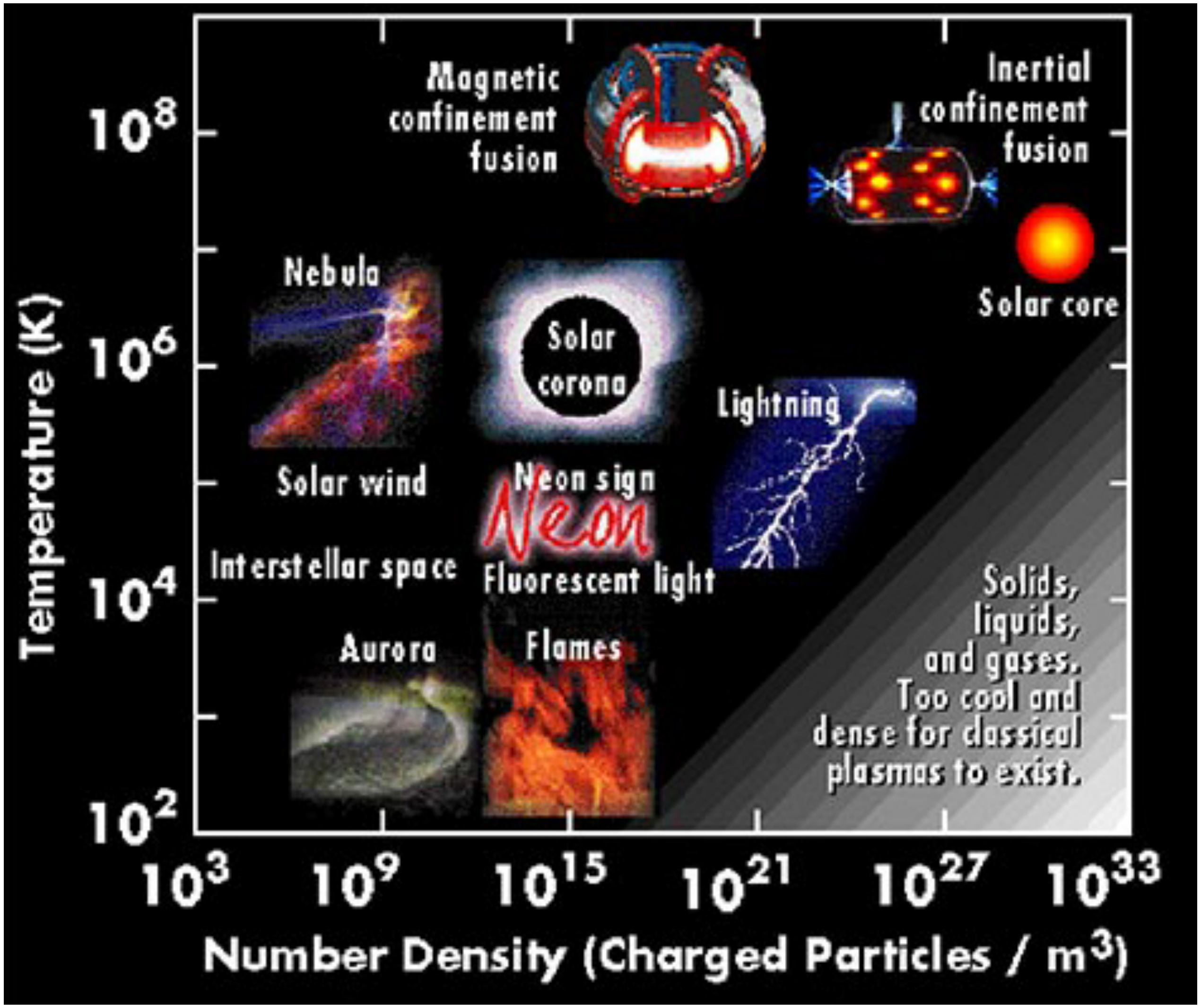
How does ICF work?



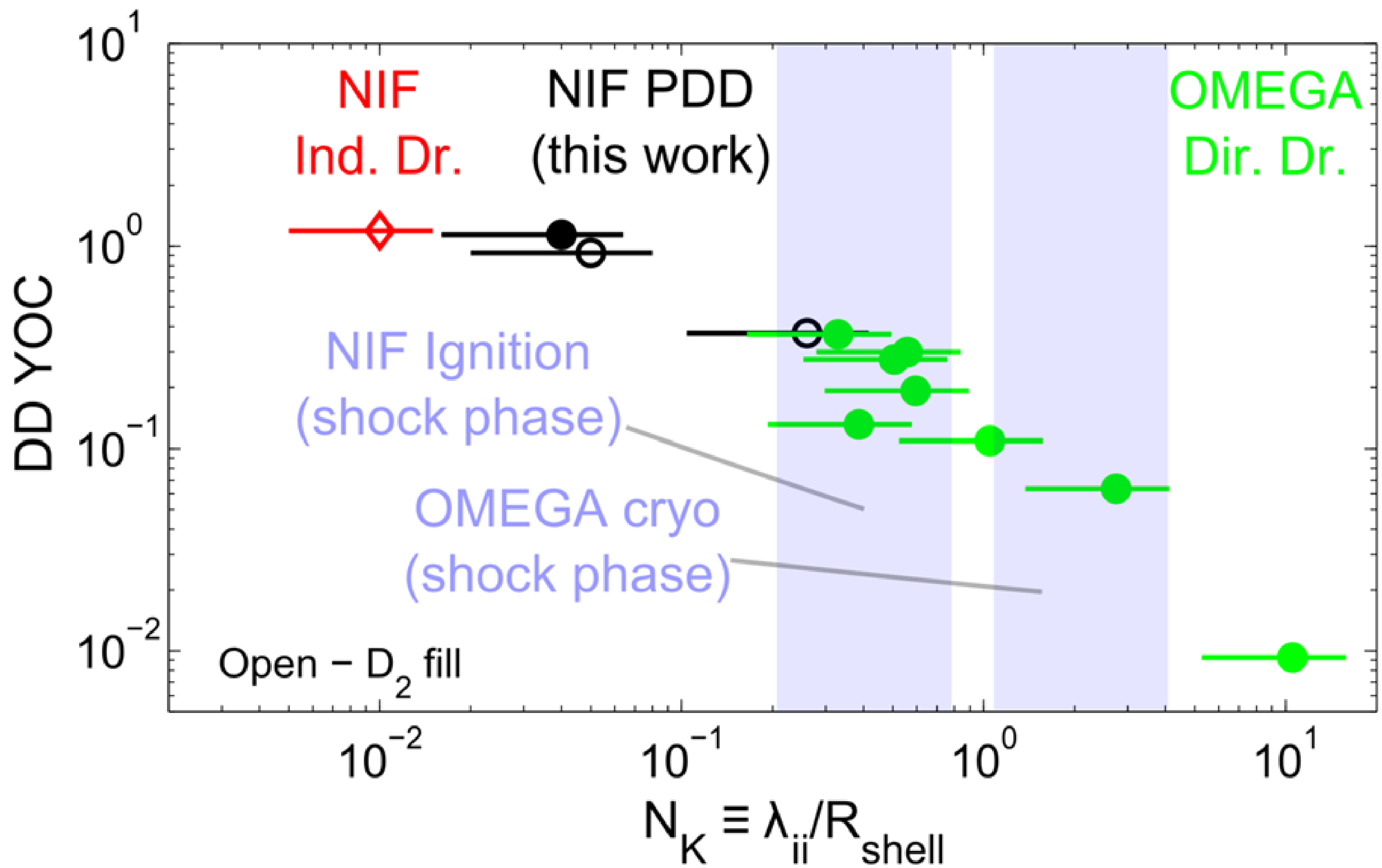




How does ICF work?



Motivation: kinetic effects in ICF are important



From Rosenberg et al., PoP, **21** (2014)

Motivation (cont.)

- **To enable kinetic simulations of full ICF spherical implosions, from early time to hot spot formation and disassembly.**
  - Kinetic effects might be important in key stages of ICF implosions (e.g., shock phase, hot-spot formation); $N_k \geq 10^{-1}$
  - Several kinetic effects have been recently suggested as potentially impacting reactivity: Knudsen layer, fuel stratification, shock broadening, kinetic interface mix,…
- **Ultimate role must be discriminated with fully kinetic (Vlasov-Fokker-Planck) simulations.**
- **A credible system-scale VFP simulation capability requires enabling algorithmic developments.**
  - Our implementation follows the multiscale philosophy of early practitioners, but with a very different implementation strategy (fully implicit, strict conservation for asymptotic well-posedness).

High-fidelity simulations require a kinetic treatment

- **Vlasov-Fokker-Planck (Rosenbluth form; equivalent to Landau form) is the model of choice for weakly coupled plasmas**

$$\frac{Df_i}{Dt} \equiv \frac{\partial f_i}{\partial t} + \vec{v} \cdot \nabla f_i + \vec{a}_i \cdot \nabla_v f_i = \sum_j \boxed{C_{ij}\left(f_i, f_j\right)}$$

$$\boxed{C_{ij}\left(f_i, f_j\right)} = \Gamma_{ij} \nabla_v \cdot \left[\boxed{D_j} \cdot \nabla_v f_i - \frac{m_i}{m_j} \boxed{A_j} f_i \right]$$

$$\boxed{D_j} = \nabla_v \nabla_v \boxed{G_j} \qquad \boxed{A_j} = \nabla_v \boxed{H_j}$$

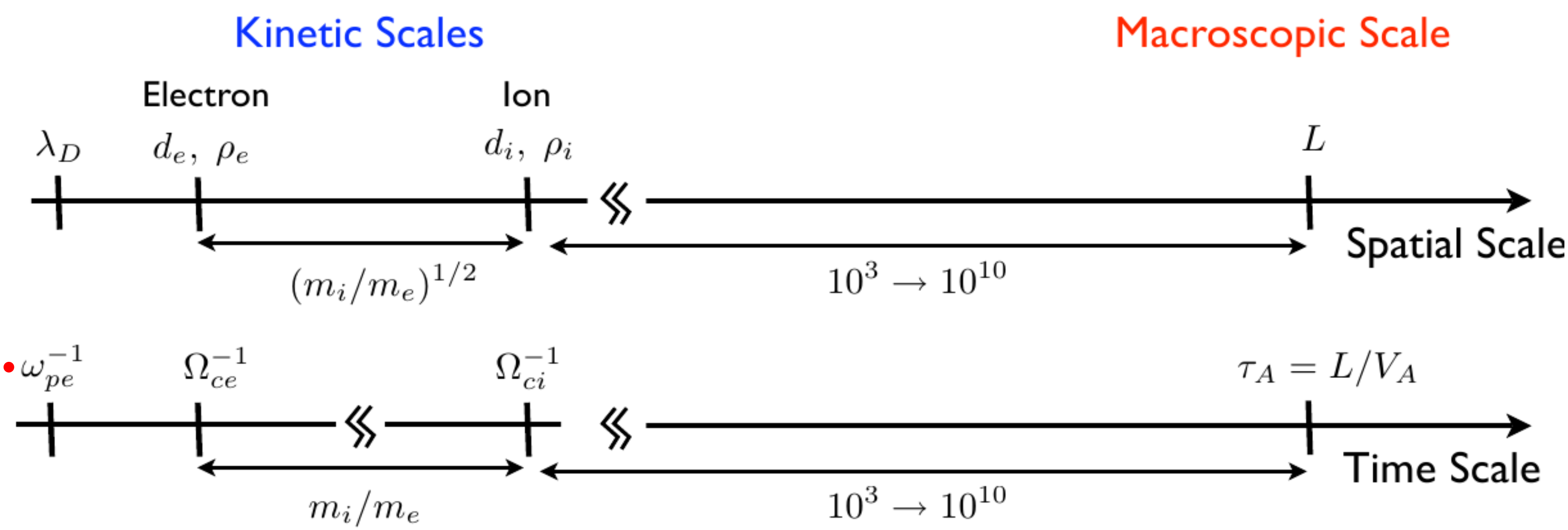
$$\nabla_v^2 \boxed{H_j} \left(\vec{v}\right) = -8\pi f_j\left(\vec{v}\right)$$

$$\nabla_v^2 \boxed{G_j} \left(\vec{v}\right) = H_j\left(\vec{v}\right)$$

+ electrons + Maxwell's equations…

VFP+Maxwell is an extremely challenging equation set

- High dimensionality (3D+3V)
- Nonlinear
- Exceedingly multiscale



The iFP Vlasov-Fokker-Planck code

A multiscale VFP solver for ICF applications

- **Consider 1D-2V geometries (planar, spherical symmetry)**
- **Consider suitable asymptotic limits for Maxwell equations:**
  - Electrostatic approximation (exact in 1D, $\beta \sim 10^3$-10^4 in Omega)
  - Quasineutrality: $\rho = 0$
  - Ambipolarity: $j = 0$ (in 1D)
  - Eliminates plasma frequency, Debye length, and charge separation effects (this is OK for our timescales)
- **Consider fluid electrons:**
  - Rigorous model, including thermal and friction forces (Simakov et al, PoP 2014)
  - Massless electrons (regular limit)
  - Eliminates non-local heat transport effects (drawback)
  - Interim approximation (ambipolarity can be imposed with kinetic e)
- **Ions remain fully kinetic, allow for multiple species**

Model equations: fully kinetic ions + fluid electrons

Vlasov-Fokker-Planck for ion species

Fluid electrons

$$\frac{3}{2}\partial_t\left(n_e T_e\right)+\frac{5}{2}\partial_x\left(u_e n_e T_e\right)-u_e\partial_x\left(n_e T_e\right)-\partial_x\kappa_e\partial_x T_e=\sum_\alpha C_{e\alpha}$$

$$n_e=-q_e^{-1}\sum^{N_s} q_\alpha n_\alpha \qquad u_e=-q_e^{-1}n_e^{-1}\sum_{\alpha\neq e}^{N_s} q_\alpha n_\alpha u_\alpha$$

Electric field model: e pressure, friction, thermal forces

$$E=-\frac{\nabla p_e+\sum_i \mathbf{F}_{ie}}{e n_e}=-\frac{\nabla p_e}{e n_e}-\frac{\alpha_0(Z_{eff})m_e}{e}\sum_i \nu_{ei}(\mathbf{V}_e-\mathbf{V}_i)-\frac{\beta_0(Z_{eff})}{e}\nabla T_e$$

Simakov and Molvig, PoP **21** (2014)

ICF kinetic simulation tools are sparse

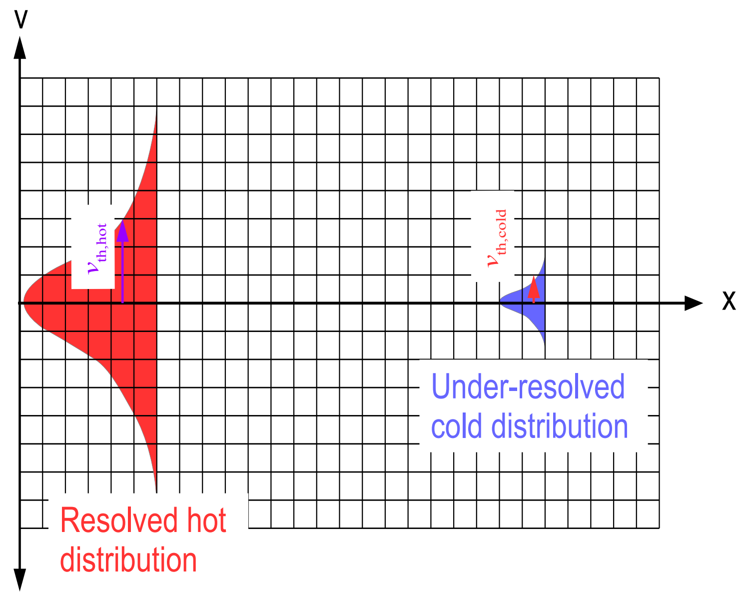
- **French CEA's FPion and FUSE code [*O. Larroche, EPJ, 27 (2003)*]:**
  - Semi-implicit ($\Delta t < \tau_{col}$ e.g. can't study pusher mix)
  - Adaptive grid, but non-conservative
    - Periodic remapping
    - Cannot investigate large mass disparities
- **Recent implosion calculations using the LSP code [*T.J.T. Kwan et al., poster, IFSA2015 (2015); A. Le et al, Phys. Plasmas, 2*]**
  - Hybrid PIC code + Monte Carlo collision operator
  - Inherits Monte Carlo limitations in convergence and order of accuracy ($\sim \mathcal{O}\left(\sqrt{\Delta t}\right)$, $\mathcal{O}(1/\sqrt{N_p})$)
  - Issues with energy conservation [*A. Le et al. KEW, LLNL (2015)*]

Algorithmic innovations of iFP

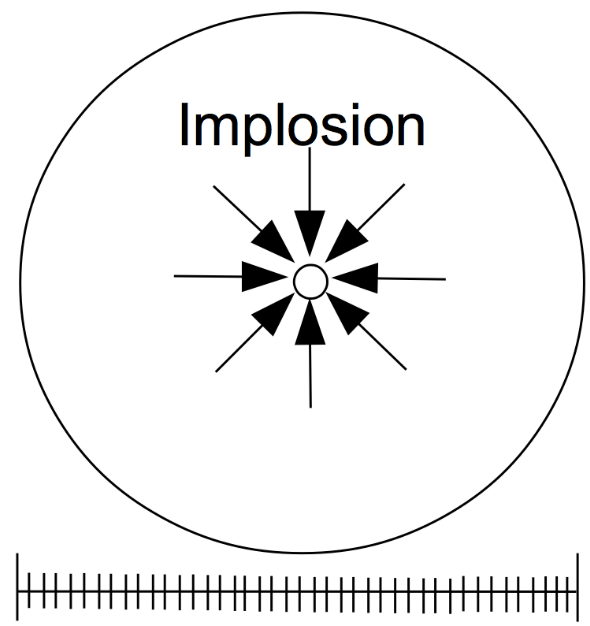
- **Fully nonlinearly time-implicit ($\Delta t \gg \tau_{col}$)**
  - Iterate solution to convergence
  - Based on an optimal multigrid preconditioned NK and AA
- **Optimal, adaptive grid in phase space**
  - Physics based adaptivity in velocity space based on characteristic normalization
  - Optimal moving mesh in physical space
- **Fully conservative (mass, momentum, and energy) and asymptotic preserving**
  - Enslavement of error in conservation symmetry into discretization

ICF adaptive meshing VFP needs

- Disparate temperatures during implosion dictate velocity resolution.
  - $v_{th,max}$ determines L_v
  - $v_{th,min}$ determines Δv



- Shock width and capsule size dictate physical space resolution



Brute-force VFP algorithms (uniform mesh, explicit timestepping) are impractical for ICF

- **Mesh requirements:**
  - Intra species $v_{th,max} / v_{th,min} \sim 100$
  - Inter species $(v_{th,\alpha} / v_{th,\beta})_{max} \sim 30$
  - $N_v \sim [10(v_{th,max}/v_{th,min}) \mathrm{x} (v_{th,\alpha} / v_{th,\beta})]^2 \sim 10^9$
  - $N_r \sim 10^3\text{-}10^4$
  - **$N=N_r N_v \sim 10^{12}\text{-}10^{13}$ unknowns in 1D2V!**
- **Timestep requirements:**
  - t_{sim}=10 ns
  - **$N_t = 10^{10}$ time steps**

$$\Delta t_{exp}^{coll} \sim \frac{1}{10} \left(\frac{\Delta v}{v_{th}^{min}} \right)^2 \nu_{coll}^{-1} \sim 10^{-9}\, ns$$

- **Beyond exascale (10^{18} FLOPS)!**

Adaptive mesh with implicit timestepping makes problem tractable

- **Mesh requirements:** $\widehat{v} = v/v_{th}$
  - v-space adaptivity with v_{th} normalization, $N_v \sim 10^4 - 10^5$
  - Moving mesh in physical space, $N_r \sim 10^2$
  - Second-order accurate phase-space discretization
  - **$N = N_v N_r \sim 10^6 \sim 10^7$** (vs. 10^{12} with static mesh)
- **Timestep requirements:**
  - Optimal $O(N_v)$ implicit nonlinear algorithms [Chacon, *JCP,* 157 (2000), Taitano et al., *JCP,* 297 (2015)]
  - Second-order accurate timestepping
  - $\Delta t_{imp} = \Delta t_{str} \sim 10^{-3}$ ns
  - **$N_t \sim 10^3 - 10^4$** (vs. 10^{10} with explicit methods)
- **Terascale-ready! (10^{12} FLOPS, any reasonable cluster)**

v_{th} adaptivity provides an enabling capability to simulate ICF plasmas

- **D-e-α, 3 species thermalization problem**
- **Resolution with static grid:**

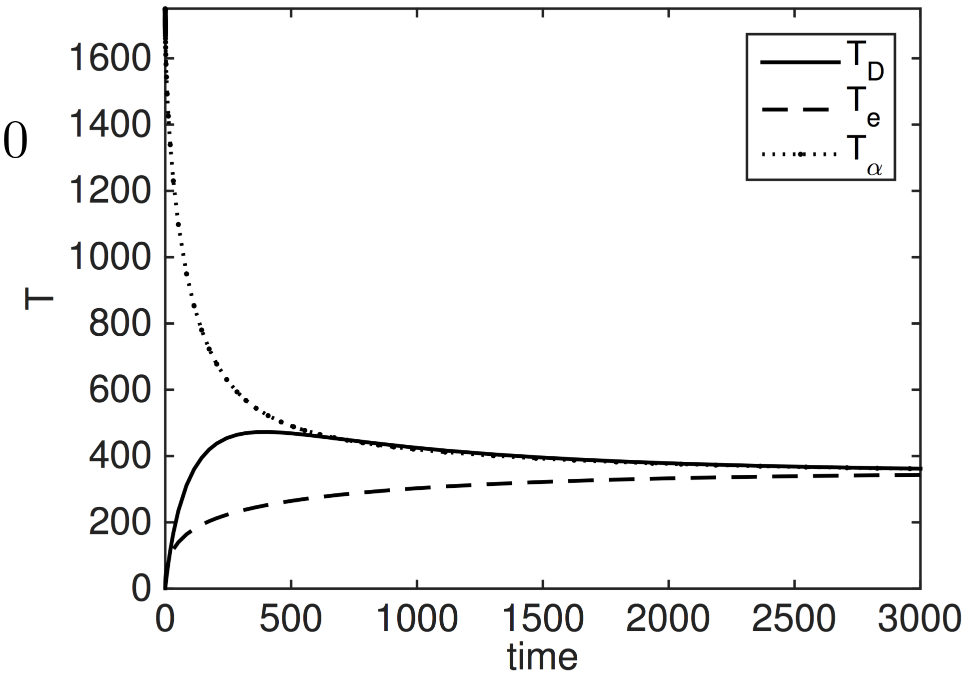
$$N_v \sim 2\left(\frac{v_{th,e,\infty}}{v_{th,D,0}}\right)^2 = 140000 \times 70000$$

- **Resolution with adaptivity and asymptotics:**

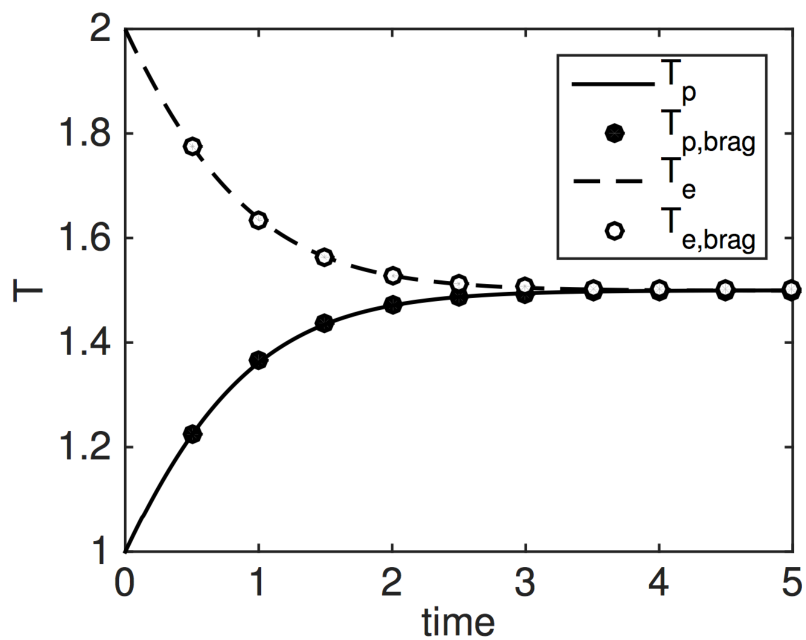
$$N_v = 128 \times 64$$

- **Mesh savings of**

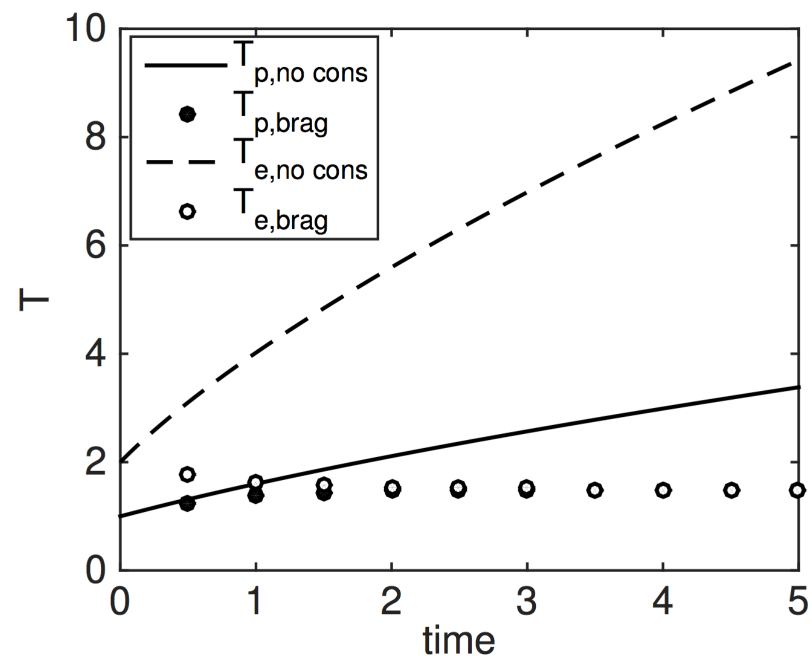
$$\sim 10^6$$



Conservation of invariants is critical!



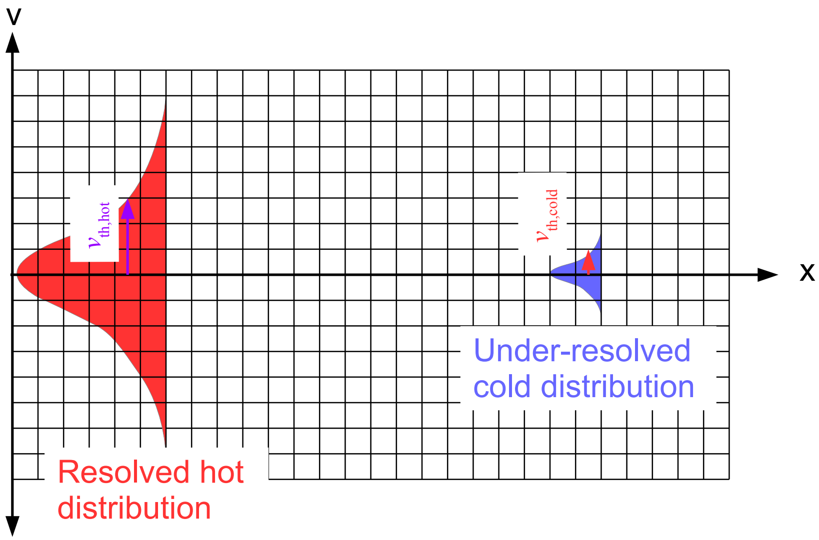
With energy conservation



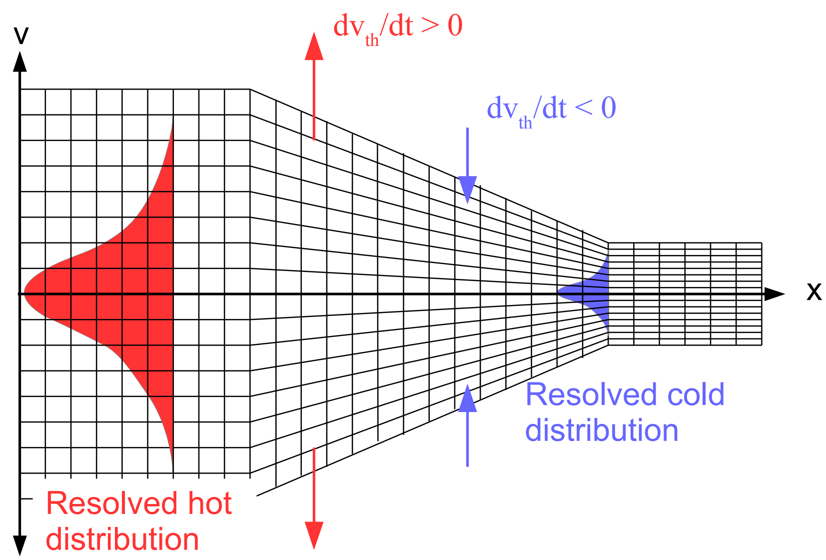
Without energy conservation

Formulation of iFP

1D-2V Rosenbluth-VFP model: Adaptive velocity space mesh



Static Mesh

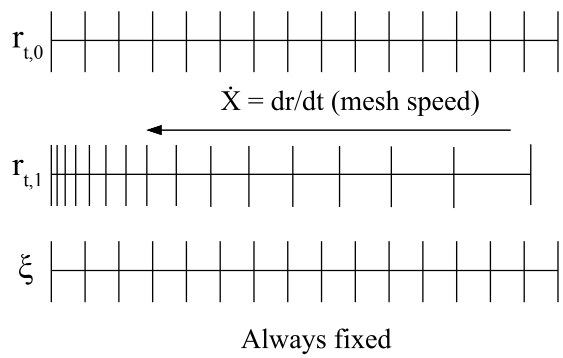


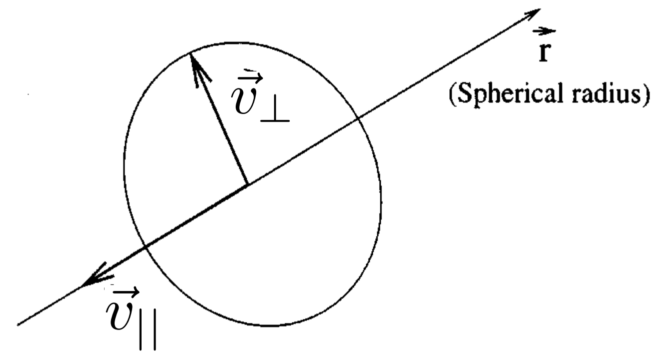
v_{th} Dynamic Mesh

- v_{th} **adaptivity allows optimal mesh resolution throughout the domain**
- **Analytical transformation introduces inertial terms**

Representation and analytical coordinate transformation for adaptive meshing

1D spherical (with logical mesh); 2D cylindrical geometry in velocity space





Coordinate transformation:

$$\widehat{v}_{||} \equiv \frac{\vec{v}\cdot\vec{\widehat{r}}}{\boxed{v_{th,\alpha}}}, \quad \widehat{v}_{\perp} \equiv \frac{\sqrt{v^2 - v_{||}^2}}{\boxed{v_{th,\alpha}}}$$

Jacobian of transformation:

$$\sqrt{g_v}\left(t, r, \widehat{v}_\perp\right) \equiv v_{th,\alpha}^3\left(t, r\right) r^2 \widehat{v}_\perp$$

$$J_{r\xi} = \partial_\xi r$$

Coordinate transformation introduces inertial terms

- **VRFP equation in transformed coordinates**

$$\partial_t \left(\sqrt{g_v} J_{r\xi} f_\alpha\right) + \partial_\xi \left(\sqrt{g_v} v_{th,\alpha} \left[\widehat{v}_{||} - \boxed{\widehat{\dot{r}}_\alpha}\right] f_\alpha\right) +$$

$$\partial_{\widehat{v}_{||}} \left(J_{r\xi}\sqrt{g_v} \boxed{\widehat{\dot{v}}_{||}} f_\alpha\right) + \partial_{\widehat{v}_\perp} \left(J_{r\xi}\sqrt{g_v} \boxed{\widehat{\dot{v}}_\perp} f_\alpha\right) = J_{r\xi}\sqrt{g_v} \sum_\beta^{N_s} C_{\alpha\beta}\left(f_\alpha, f_\beta\right)$$

$$\boxed{\widehat{\dot{v}}_{||}} = \boxed{-\frac{\widehat{v}_{||}}{2}\left(v_{th,\alpha}^{-2}\partial_t v_{th,\alpha}^2 + J_{r\xi}^{-1}\left(\widehat{v}_{||} - \widehat{\dot{x}}\right) v_{th,\alpha}^{-1}\partial_\xi v_{th,\alpha}^2\right)} + \frac{\widehat{v}_\perp^2 v_{th,\alpha}}{r} + \frac{q_\alpha E_{||}}{J_{r\xi} m_\alpha v_{th,\alpha}}$$

$$\boxed{\widehat{\dot{v}}_\perp} = \boxed{-\frac{\widehat{v}_\perp}{2}\left(v_{th,\alpha}^{-2}\partial_t v_{th,\alpha}^2 + J_{r\xi}^{-1}\left(\widehat{v}_{||} - \widehat{\dot{x}}\right) v_{th,\alpha}^{-1}\partial_\xi v_{th,\alpha}^2\right)} \frac{\widehat{v}_{||}\widehat{v}_\perp v_{th,\alpha}}{r}$$

Inertial terms due to v_{th} adaptivity and Lagrangian mesh

Taitano, JCP, 318, 2016
Taitano, JCP, 2017, submitted

Implicit solver strategy:
Preconditioned Anderson Acceleration

- **Define the nonlinear residual:**

$$R = \partial_t f + VE(f) - \nabla_v \cdot [\underline{\underline{D}} \cdot \nabla_v f - \underline{A} f] = 0$$

- **Consider fixed-point map:** $G(f_k) = f_k - P_k^{-1} R_k = f_{k+1}$
  - If $P_k = J_k$, we recover Newton's method
- **Anderson updates the solution by using history (nonlinear) of solutions to accelerate convergence via:**

$$f_{k+1} = \sum_{i=0}^{m_k} \alpha_i^{(k)} G\left(f_{k-m_k+i}\right)$$

- **Can be readily preconditioned (** P_k^{-1} **)**
- **Suitable for use with non-differentiable residuals (limiters, etc)**

D. G. Anderson. Iterative procedures for nonlinear integral equations. *J. Assoc. Comput. Machinery*, 12:547–560, 1965.

Two stage operator splitting in PC operator

$$P^{-1}R = P_x^{-1}P_v^{-1}R$$

Step 1: Velocity space operators (including collisions)

$$P_v \circ = \partial_t \circ + V E_v(\circ) - \nabla_v \cdot [\underline{\underline{D}} \cdot \nabla_v \circ - \underline{A} \circ]$$

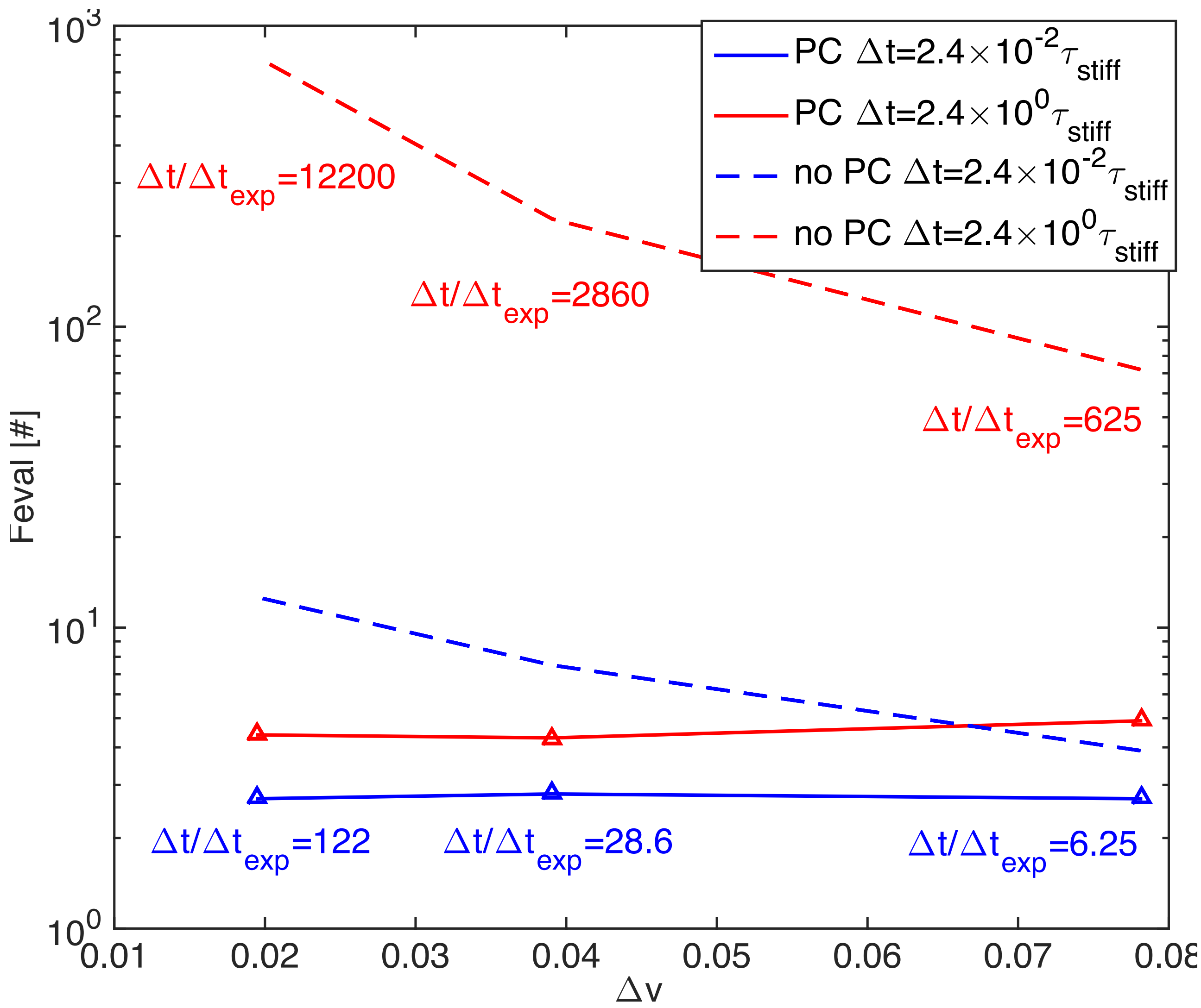
Step 2: Streaming operator

$$P_x \circ = \partial_t \circ + \partial_x \circ$$

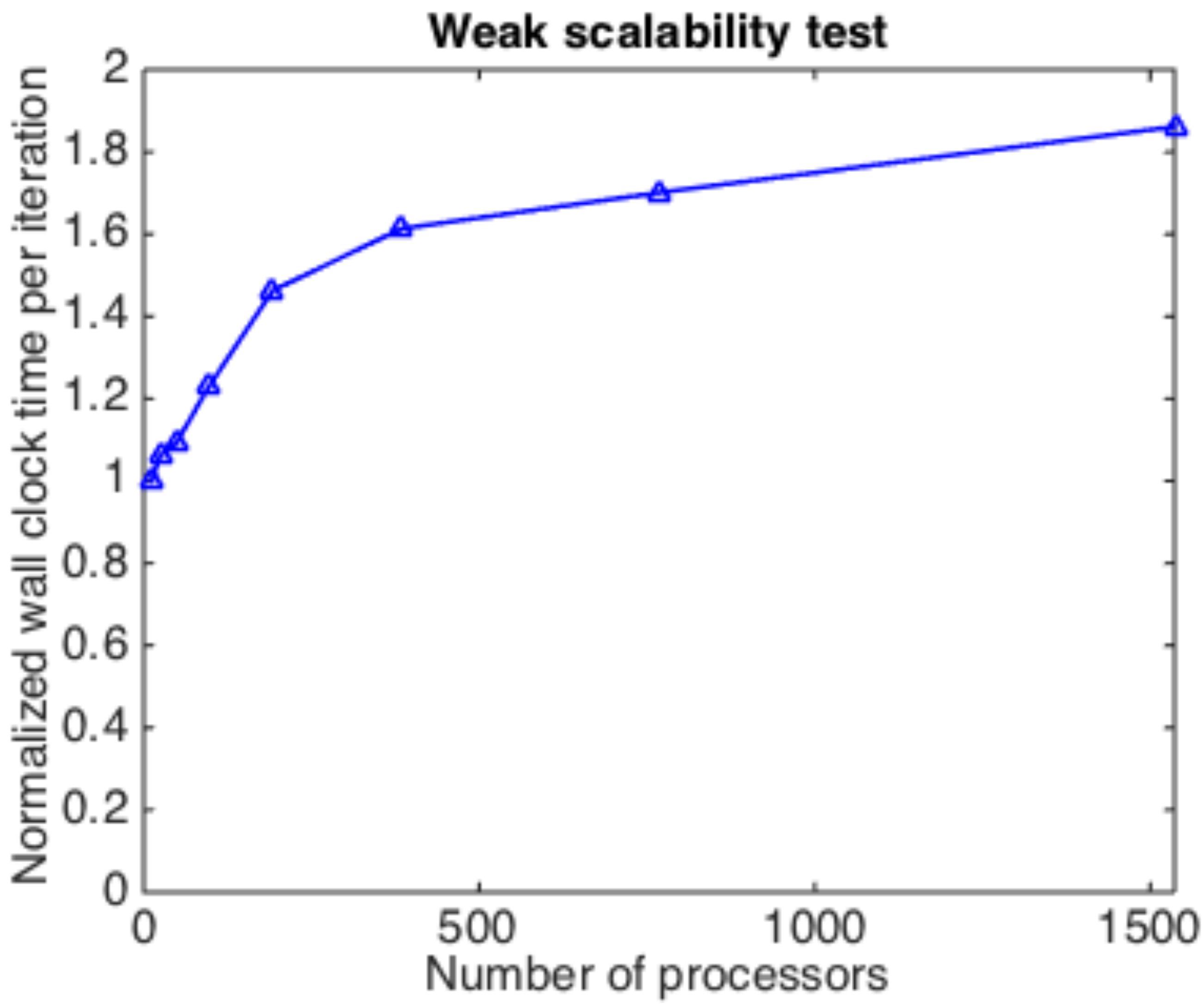
Preconditioner is an *accelerator* of convergence!

No splitting error will be present in the actual solution (driven by the nonlinear residual)

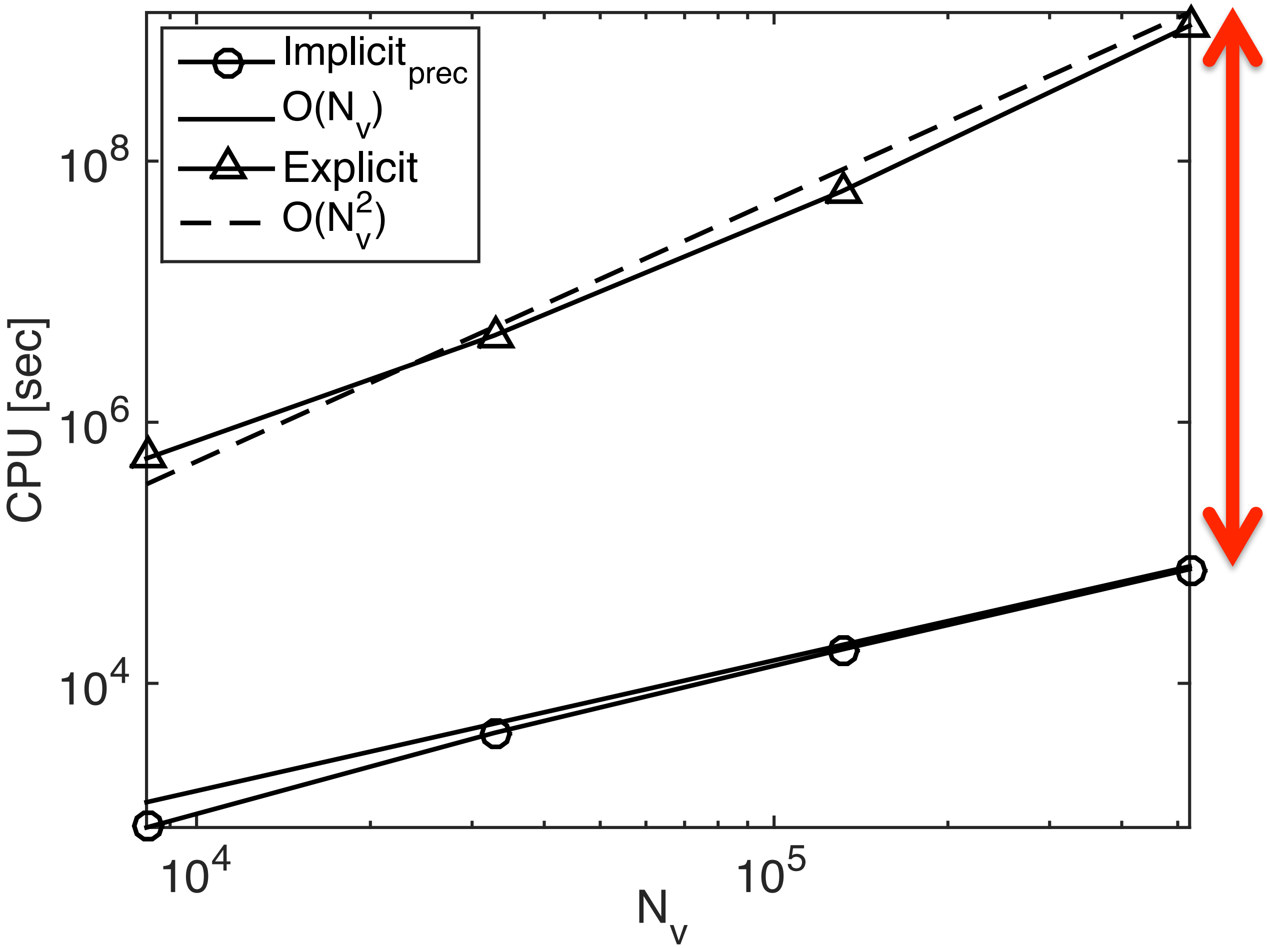
Nonlinear solver is algorithmically scalable, $O(N_v)$



Algorithm is highly scalable in parallel, $O(N_p)$

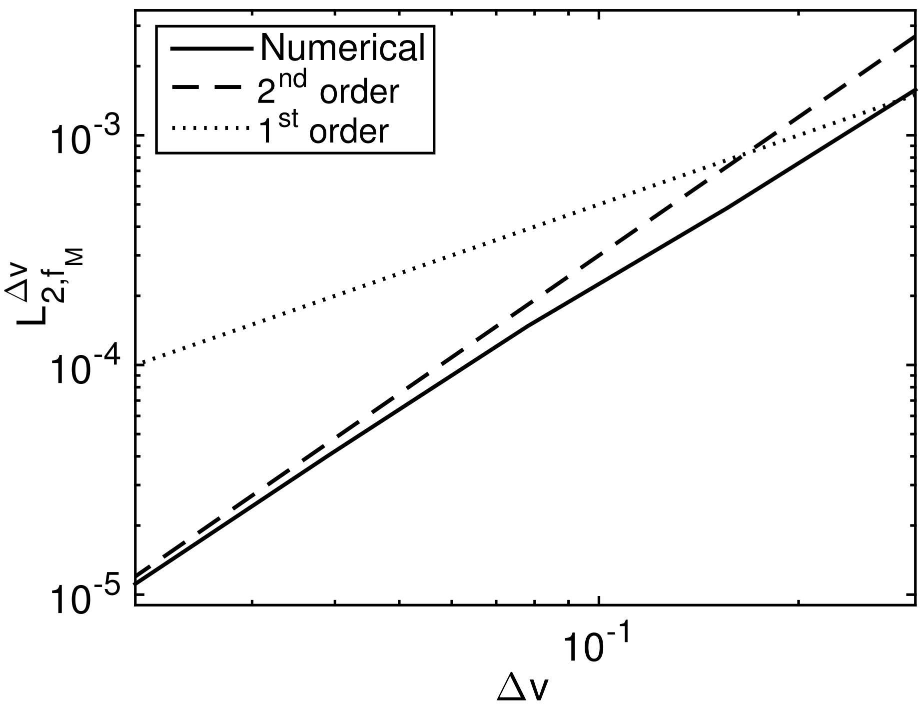


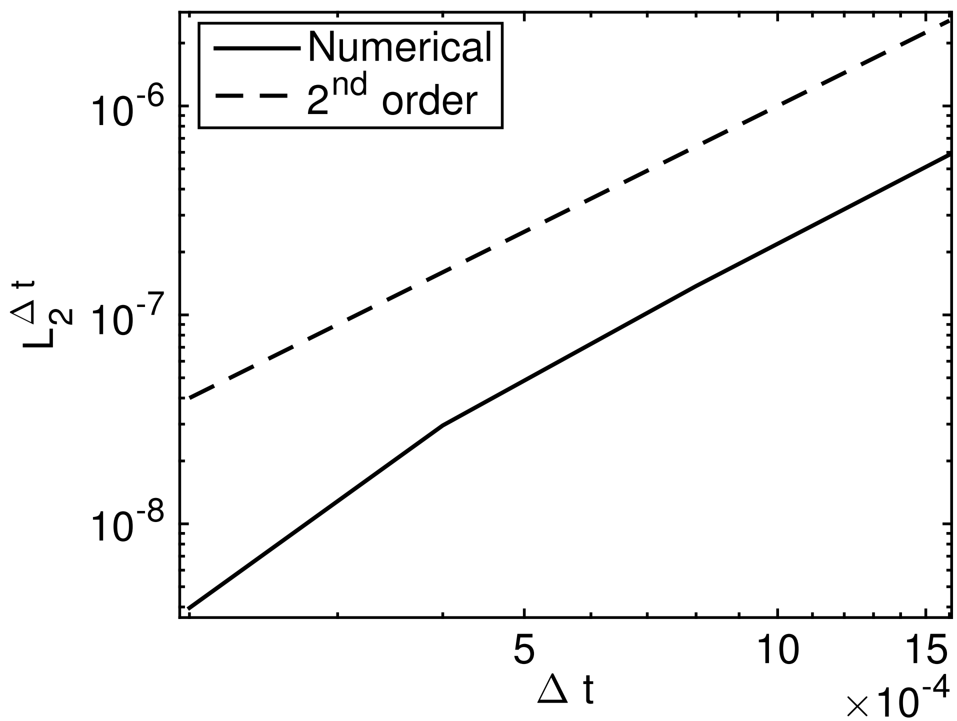
Implicit solver is very efficient



4 orders of magnitude more efficient than explicit methods

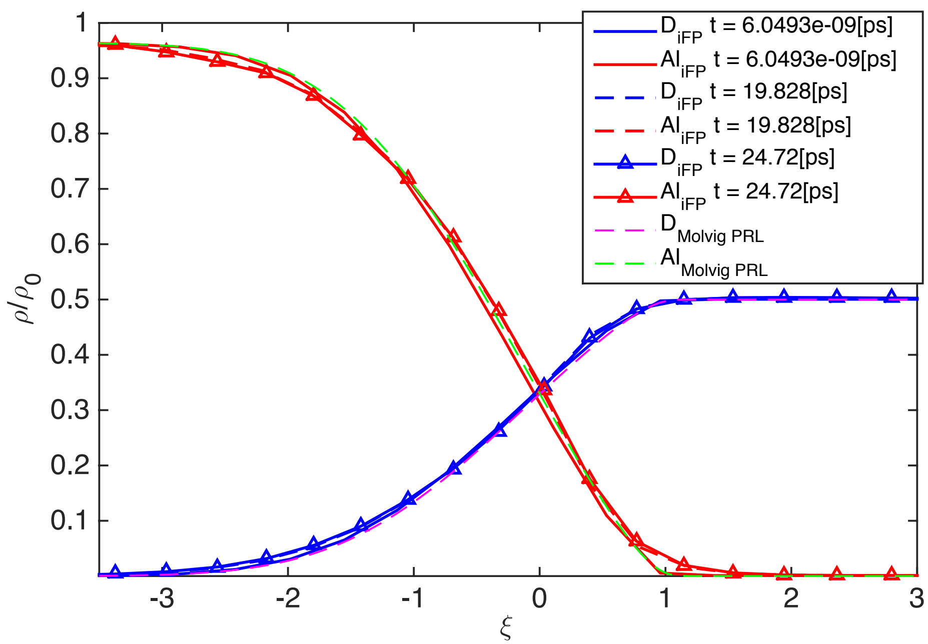
Algorithm achieves design accuracy (2nd order spatially and temporally)

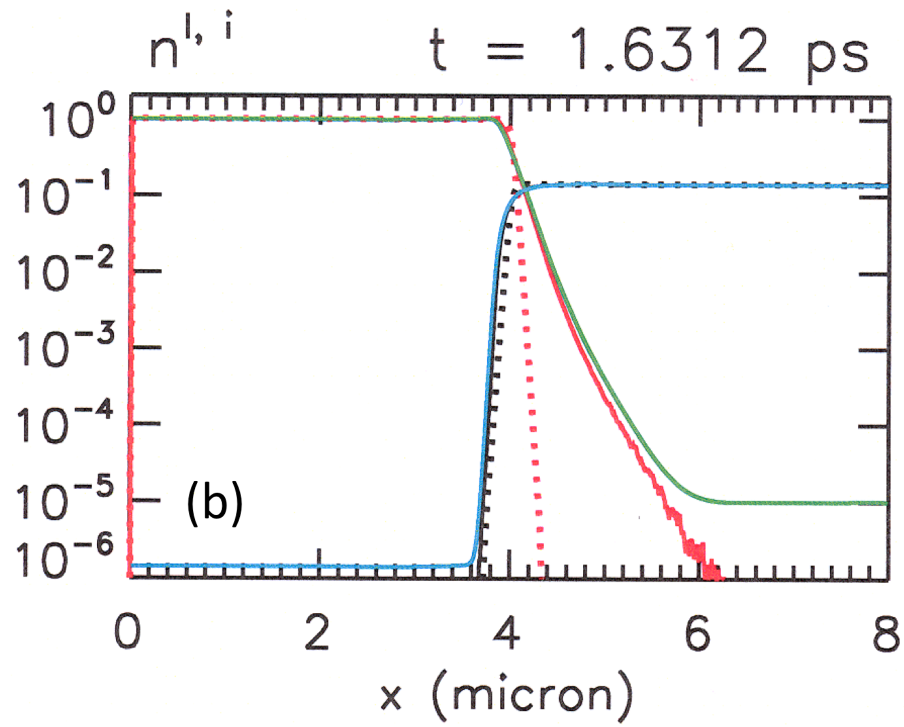




Algorithm is highly accurate even when $\Delta t >> \tau_{col}$

- Correct self-similar solution [*K. Molvig et al., PRL 113 (2014)*] obtained for $t >> \tau_{col}$
- Test of implicit solver with $\Delta t = 4 \times 10^4 \tau_{col}$
- Successfully benchmarked against the DSMC VPIC code [Yin et al, *Phys. Plasmas*, 2016]





Rosenbluth-Fokker-Planck collision operator: Velocity Space Adapativity

1D-2V Rosenbluth-VFP model: analytical velocity space adaptivity (cont.)

Normalization of collision operator

$$\widehat{C}_{\alpha\beta} = \boxed{v_{th,\alpha}^3} C_{\alpha\beta}$$

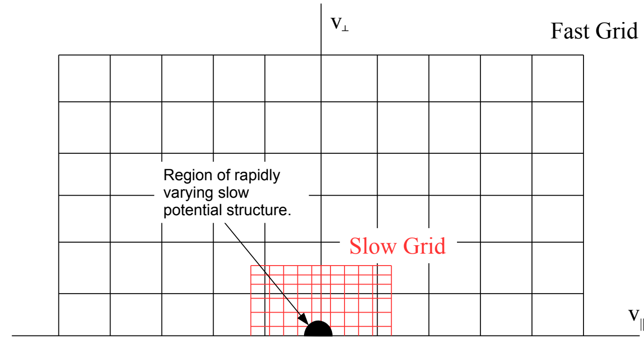
$$\boxed{\widehat{C}_{\alpha\beta} = \frac{\Gamma_{\alpha\beta}}{v_{th,\beta}^3} \widehat{\nabla}_{v_\alpha} \cdot \left[\widehat{\nabla}_{v_\alpha} \widehat{\nabla}_{v_\alpha} \widehat{G}_{\alpha\beta} \cdot \widehat{\nabla}_{v_\alpha} \widehat{f}_\alpha - \frac{m_\alpha}{m_\beta} \widehat{f}_\alpha \widehat{\nabla}_{v_\alpha} \widehat{H}_{\alpha\beta} \right]}$$

$$\widehat{\nabla}_{v_\alpha}^2 \widehat{H}_{\alpha\beta} = -8\pi \boxed{\widehat{f}_\beta \left(\widehat{v}_\beta = \widehat{v}_\alpha \frac{v_{th,\alpha}}{v_{th,\beta}} \right)} \qquad \widehat{\nabla}_{v_\alpha}^2 \widehat{G}_{\alpha\beta} = \widehat{H}_{\alpha\beta}$$

$$\hat{H}_{\alpha\beta} = H_\beta \frac{v_{th,\beta}^3}{v_{th,\alpha}^2} \qquad \hat{G}_{\alpha\beta} = G_\beta \frac{v_{th,\beta}^3}{v_{th,\alpha}^4}$$

Procedure requires a transfer operation of $\widehat{f}_\beta$ to $\hat{v}_\alpha$ space, which can be problematic when $\hat{v}_\alpha \gg \hat{v}_\beta \quad \text{or} \quad \hat{v}_\beta \gg \hat{v}_\alpha$: asymptotic treatment

Velocity space adaption does not help for interspecies collisions



- **For electron-ion collisions, $v_{th,e}/v_{th,i} >> 1$**
- **Similarly, for α-ion collisions, $v_{th,\alpha}/v_{th,I} >> 1$**
- **Very stringent mesh resolution requirements if determining potentials via:**

$$\nabla_v^2 H_j(\vec{v}) = -8\pi f_j(\vec{v}) \qquad \nabla_v^2 G_j(\vec{v}) = H_j(\vec{v})$$

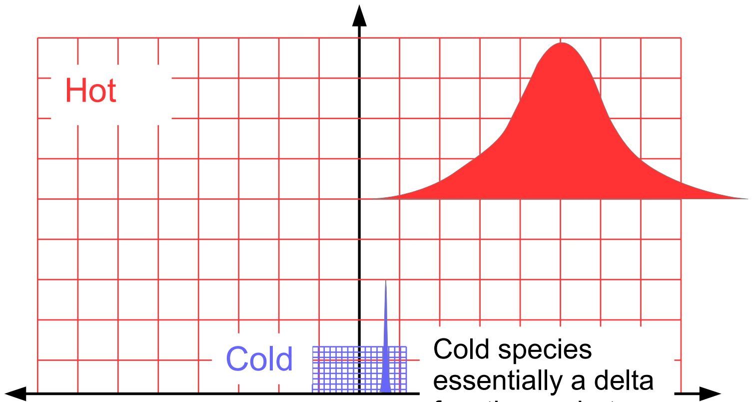
- **Mesh requirement grows as:**

$$N_v^d \propto \left(\frac{v_{th,f}}{v_{th,s}}\right)^d$$

- **Velocity space adaption helps ONLY for self-species, but not for interspecies! We need an asymptotic treatment**

1D-2V Rosenbluth-VFP model: Asymptotic Formulation of Interspecies Collisions for $v_{th,f} >> v_{th,s}$

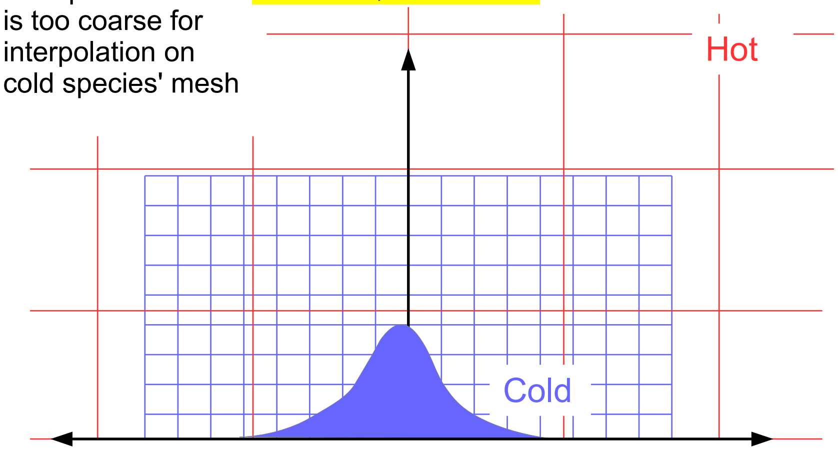
$v_f/v_{th,s} >> 1$



$$H_s = \frac{n_s}{v} + \frac{n_s \boldsymbol{V}_s \cdot \boldsymbol{v}}{v^3} + \cdots$$

$$G_s = n_s v - \frac{n_s \boldsymbol{V}_s \cdot \boldsymbol{v}}{v} + \nabla_v \nabla_v v : \left(\frac{1}{2} \int \mathrm{d}^3 v' \, f_s' \boldsymbol{v}' \boldsymbol{v}' \right) + \cdots$$

$v_s/v_{th,f} << 1$



$$H_f = \boldsymbol{v} \cdot \left(\int \mathrm{d}^3 v' \, f_f' \frac{\boldsymbol{v}'}{v'^3} \right) + \frac{1}{2} \boldsymbol{vv} : \left[\int \mathrm{d}^3 v' \, f_f' \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right]$$
$$- \frac{1}{6} \boldsymbol{vvv} \vdots \left[\int \mathrm{d}^3 v' \, f_f' \nabla_{v'} \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right]$$
$$+ \frac{1}{24} \boldsymbol{vvvv} :: \left[\int \mathrm{d}^3 v' \, f_f' \nabla_{v'} \nabla_{v'} \nabla_{v'} \nabla_{v'} \left(\frac{1}{v'} \right) \right] + \cdots$$

$$G_f = \frac{1}{2} \boldsymbol{vv} : \left(\int \mathrm{d}^3 v' \, f_f' \nabla_{v'} \nabla_{v'} v' \right) - \frac{1}{6} \boldsymbol{vvv} \vdots \left(\int \mathrm{d}^3 v' \, f_f' \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right)$$
$$+ \frac{1}{24} \boldsymbol{vvvv} :: \left(\int \mathrm{d}^3 v' \, f_f' \nabla_{v'} \nabla_{v'} \nabla_{v'} \nabla_{v'} v' \right) + \cdots$$

Rosenbluth-Fokker-Planck collision operator: conservation of mass, momentum, and energy

2V Rosenbluth-FP collision operator: conservation properties

- **Conservation properties of FP collision operator result from symmetries:**

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

Mass

$$\langle 1, C_{\alpha\beta} \rangle_{\vec{v}} = 0 \quad \Rightarrow \quad \boxed{\left. \vec{J}_{\alpha\beta,G} - \vec{J}_{\alpha\beta,H} \right|_{\partial \vec{v}} = 0}$$

Momentum

$$m_\alpha \langle \vec{v}, C_{\alpha\beta} \rangle_{\vec{v}} = -m_\beta \langle \vec{v}, C_{\beta\alpha} \rangle_{\vec{v}} \quad \Rightarrow \quad \boxed{\left\langle 1, J^{\|}_{\alpha\beta,G} - J^{\|}_{\beta\alpha,H} \right\rangle_{\vec{v}} = 0}$$

Energy

$$m_\alpha \left\{ \left\langle v^2, C_{\alpha\beta} \right\rangle_{\vec{v}} \right\} = -m_\beta \left\{ \left\langle v^2, C_{\beta\alpha} \right\rangle_{\vec{v}} \right\} \Rightarrow \boxed{\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0}$$

2V Rosenbluth-FP collision operator: numerical conservation of energy

- **The symmetry to enforce is:** $\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0$
- **Due to discretization error:** $\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = \boxed{\mathcal{O}\left(\Delta_v\right)}$
- **We introduce a constraint coefficient such that:**

$$\left\langle \vec{v}, \boxed{\gamma_{\beta\alpha}} \vec{J}_{\beta\alpha,G} - \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}} = 0 \qquad \gamma_{\beta\alpha} = \frac{\left\langle \vec{v}, \vec{J}_{\alpha\beta,H} \right\rangle_{\vec{v}}}{\left\langle \vec{v}, \vec{J}_{\beta\alpha,G} \right\rangle_{\vec{v}}} = 1 + \boxed{\mathcal{O}\left(\Delta_v\right)}$$

$$C_{\alpha\beta} = \Gamma_{\alpha\beta} \nabla_v \cdot \left[\boxed{\gamma_{\alpha\beta}} \vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta} \vec{J}_{\alpha\beta,H} \right]$$

- **Discretization is nonlinear, and ensures that, numerically:**

$$m_\alpha \left\{ \left\langle v^2, C_{\alpha\beta} \right\rangle_{\vec{v}} \right\} = -m_\beta \left\{ \left\langle v^2, C_{\beta\alpha} \right\rangle_{\vec{v}} \right\}$$

2V Rosenbluth-FP collision operator: numerical conservation of momentum+energy

- **Simultaneous conservation of momentum and energy requires enforcing both symmetries numerically:**

$$\boxed{C_{\alpha\beta} = \Gamma_{\alpha\beta}\nabla_v \cdot \left[\boxed{\underline{\underline{\eta}}_{\alpha\beta}} \cdot \vec{J}_{\alpha\beta,G} - \frac{m_\alpha}{m_\beta}\vec{J}_{\alpha\beta,H}\right]}$$

with:

$$\underline{\underline{\eta}}_{\alpha\beta} = \begin{bmatrix} \gamma_{\alpha\beta} + \epsilon_{||,\alpha\beta} & 0 \\ 0 & \gamma_{\alpha\beta} \end{bmatrix}$$

Momentum

Energy

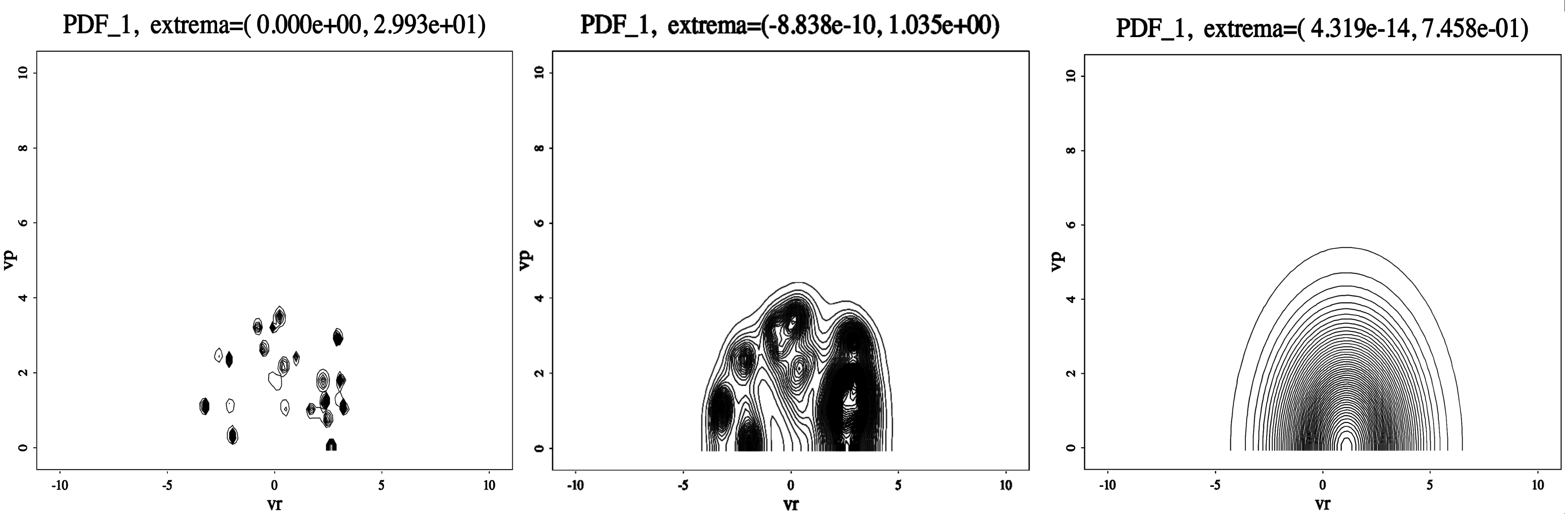
$$\gamma_{\alpha\beta} = \frac{\left\langle \vec{v}, \vec{J}_{H,\beta\alpha} \right\rangle_{\vec{v}} + \boxed{\epsilon^{+}_{\alpha\beta,||}} \left\langle \vec{v}, \vec{J}_{G,\alpha\beta} \right\rangle^{+\infty}_{\vec{v}-\vec{u}}}{\left\langle \vec{v}, \vec{J}_{G,\alpha\beta} \right\rangle_{\vec{v}}}$$

$$\epsilon_{\alpha\beta} = \left\{ \begin{array}{cc} \epsilon^{-}_{||,\alpha\beta} = 0 & \text{if } v_{||} - u_{avg,||,\alpha\beta} \leq 0 \\ \epsilon^{+}_{||,\alpha\beta} = \frac{\left\langle 1, J_{H,\beta\alpha,||} \right\rangle_{\vec{v}} + \boxed{\gamma_{\alpha\beta}} \left\langle 1, J_{G,\alpha\beta,||} \right\rangle_{\vec{v}}}{\left\langle 1, J_{G,\alpha\beta,||} \right\rangle^{+\infty}_{\vec{v}-\vec{u}_{avg,\alpha\beta}}} & \text{else} \end{array} \right\}$$

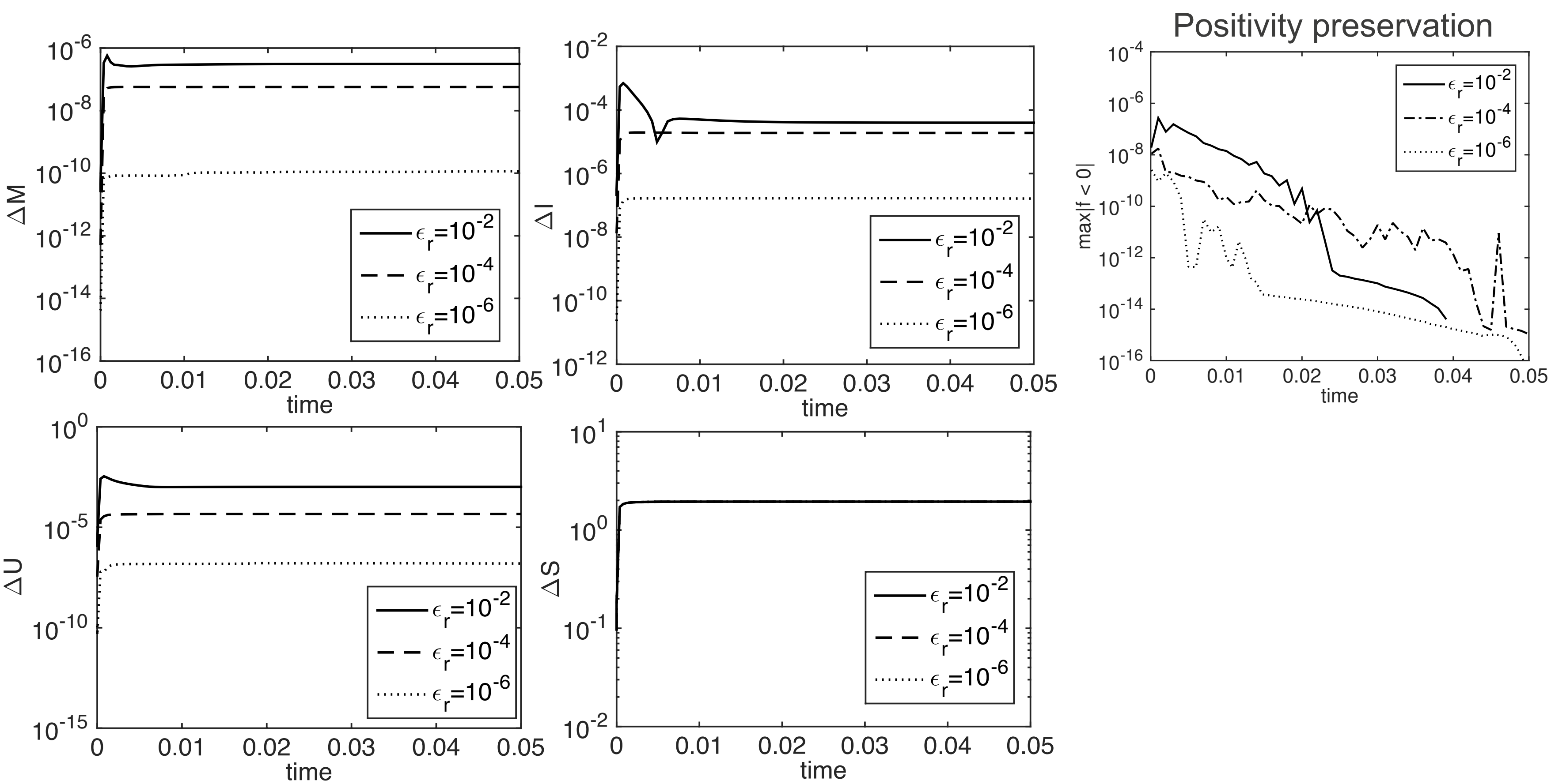
2V Rosenbluth-FP collision operator: numerical preservation of positivity

- **RFP collision operator is an advection-(tensor) diffusion operator in velocity space**
- **Use SMART (Gaskell & Law, 1988) for advection**
  - High-order advection when possible
  - Reverts to upwinding otherwise
  - Monotonic, positivity preserving
  - Suitable for implicit timestepping
- **Use limited tensor diffusion (Lipnikov et al., 2012) for tensor diffusion component**
  - Maximum-principle preserving
  - Compatible with nonlinear iterative solvers

Single-species initial random distribution: Thermalization to a Maxwellian

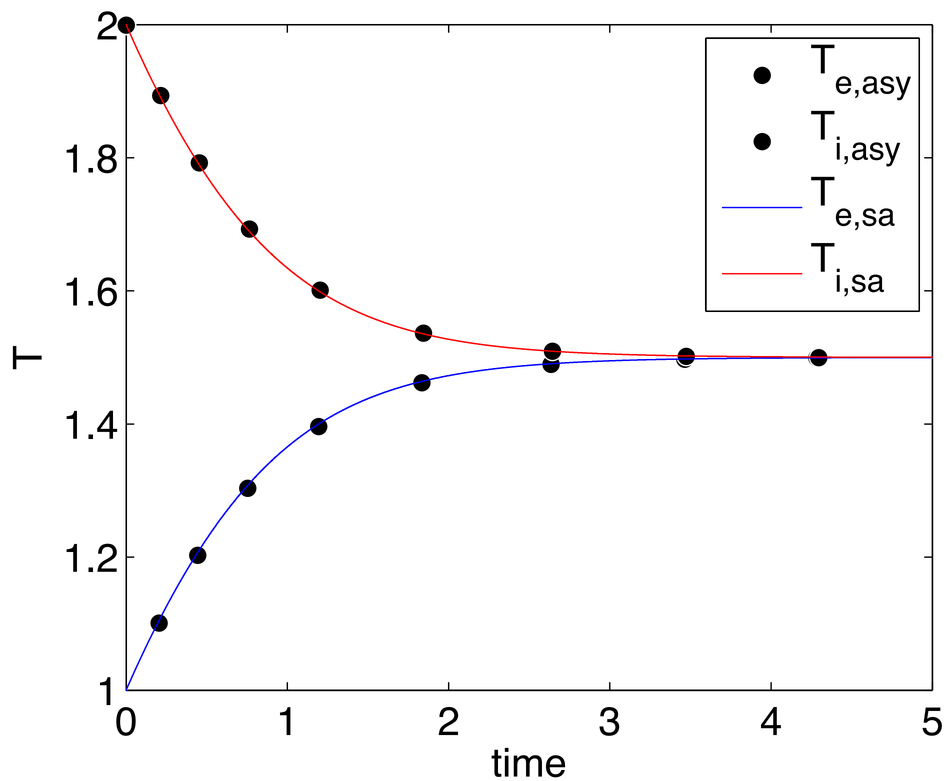


Single-species random distribution: Conservation properties



Electron-proton Temperature relaxation: Asymptotic treatment test & mesh savings

- **Realistic mass ratio, m_i/m_e = 1836**
- **Temperature disparity of 2 => $v_{th,e}$ ~ 60 $v_{th,i}$**



Mesh used with asymptotics: 128x64

Brute force (no asymptotics) will require:

$$2\left(\frac{v_{th,e}}{v_{th,i}} n_{min}\right)^2 \sim 2400 \times 1200$$

Velocity mesh savings of ~350!

v_{th} adaptivity provides an enabling capability to simulate ICF plasmas

- D-e-α, 3 species thermalization problem
- Resolution with static grid:

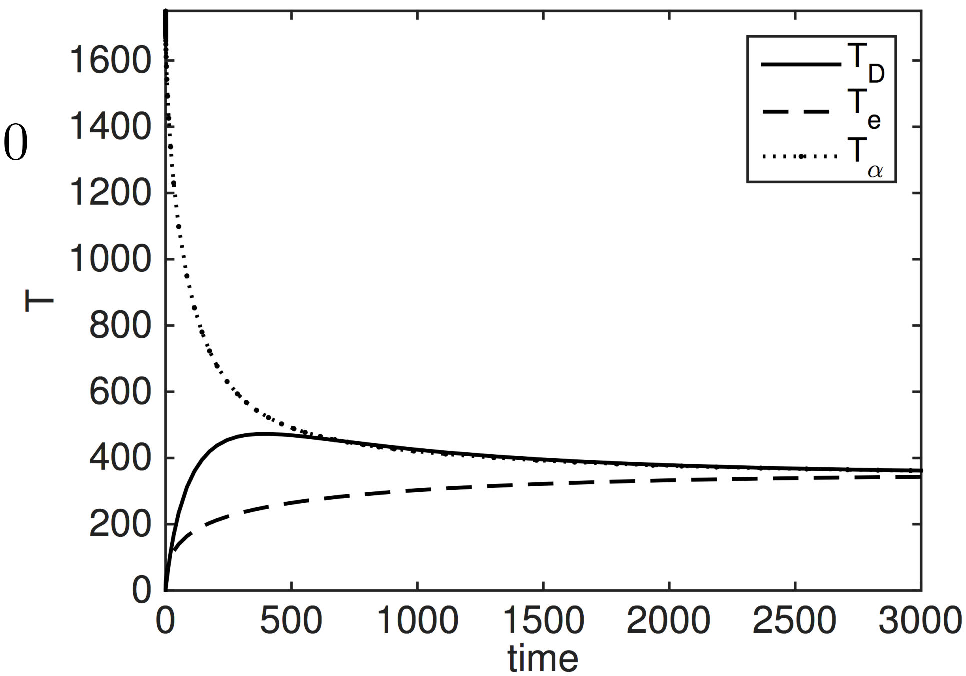
$$N_v \sim 2\left(\frac{v_{th,e,\infty}}{v_{th,D,0}}\right)^2 = 140000 \times 70000$$

- Resolution with adaptivity and asymptotics:

$$N_v = 128 \times 64$$

- Mesh savings of

$$\sim 10^6$$



1D-2V Vlasov equation: Conservation properties with velocity space adaptivity

Temporal Inertial Terms

Vlasov equation with adaptivity in velocity space: Temporal inertial terms

- Focus on temporal inertial terms due to normalization wrt $v_{th}(r,t)$ (0D):

$$\frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{1}{2}\frac{\partial \ln T_\alpha}{\partial t}\widehat{\nabla}_v \cdot \left[\vec{\widehat{v}}\widehat{f}_\alpha\right] = 0$$

- Which can be rewritten as:

$$\boxed{v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2}\widehat{\nabla}_v \cdot \left(\vec{\widehat{v}}\widehat{f}_\alpha\right) = 0}$$

- Mass conservation can be trivially shown from this equation by integrating in velocity space

$$v_{th}^2 \frac{\partial n_\alpha}{\partial t} = 0$$

VE with adaptivity in velocity space: Conservation of momentum

$$\boxed{v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) = 0}$$

- **Rewrite as:**

$$v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right] \right\} = 0$$

- **Momentum conservation can be trivially shown by taking second velocity moment and gives:**

$$v_{th} \frac{\partial (n_\alpha \vec{u}_\alpha)}{\partial t} = 0$$

- **This property relies on the fact that:** $\boxed{\left\langle \vec{\widehat{v}}, \widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0}$
- **This property must be enforced numerically:**

$$\left\langle \vec{\widehat{v}}, \widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\underline{\underline{\Upsilon}}_{t,\alpha} \vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0 \quad \underline{\underline{\Upsilon}}_{t,\alpha} = \begin{bmatrix} \Upsilon_{\parallel,\alpha} & 0 \\ 0 & 1 \end{bmatrix}$$

VE adaptivity in velocity space: Conservation of energy

$$v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) = 0$$

- Rewrite as:

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right] = 0$$

- Energy conservation can be trivially shown by taking first velocity moment and gives:

$$\frac{\partial U_\alpha}{\partial t} = 0$$

- This property relies on the fact that: $\left\langle \widehat{v}^2, \widehat{f}_\alpha + \frac{1}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0$
- This property must be enforced numerically:

$$\left\langle \widehat{v}^2, \widehat{f}_\alpha + \frac{\gamma_{t,\alpha}}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\vec{v}} = 0 \qquad \gamma_{t,\alpha} = - \frac{\left\langle \frac{\widehat{v}^2}{2}, \widehat{f}_\alpha \right\rangle_{\widehat{v}}}{\left\langle \frac{\widehat{v}^2}{2}, \frac{1}{2} \widehat{\nabla}_v \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right\rangle_{\widehat{v}}}$$

VE adaptivity in velocity space:
All conservation laws

$$v_{th,\alpha}^2 \frac{\partial \widehat{f}_\alpha}{\partial t} - \frac{\partial_t v_{th,\alpha}^2}{2} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) = 0$$

- **Rewrite as:**

Truncation error

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \gamma_{t,\alpha} \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right] + \xi_{t,\alpha} = 0$$

$$\xi_{t,\alpha} = v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\underline{\underline{\Upsilon}}_{t,\alpha} \widehat{\vec{v}} \widehat{f}_\alpha \right) \right] \right\} + \eta_{t,\alpha}$$
$$- \left\{ \partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right] \right\};$$

$$\eta_{t,\alpha}(v) = \left\{ v_{th,\alpha}^2 \partial_t \widehat{f}_\alpha - \partial_t v_{th,\alpha}^2 \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right\}$$
$$- v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha \right) \right] \right\}$$

1D Spatial Inertial Terms

VE adaptivity in velocity space:
Spatial inertial terms

- **All Coriolis terms due to normalization wrt $v_{th}(r,t)$:**

$$v_{th,\alpha}^2 \partial_t \widehat{f}_\alpha + \boxed{v_{th,\alpha}^2 \partial_x \left(v_{th,\alpha} \widehat{v}_{||} \widehat{f}_\alpha \right)} - \partial_t v_{th,\alpha}^2 \frac{\widehat{\nabla}_v}{2} \cdot \left[\vec{\widehat{v}} \widehat{f}_\alpha \right] - v_{th,\alpha} \boxed{\partial_x v_{th,\alpha}^2} \frac{\widehat{\nabla}_v}{2} \cdot \left[\vec{\widehat{v}} \widehat{v}_{||} \widehat{f}_\alpha \right] = 0$$

- **Conservation of momentum:**

$$v_{th,\alpha} \left\{ \partial_t \left(v_{th,\alpha} \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha} \left[\widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\underline{\underline{\Upsilon}}_{t,\alpha} \vec{\widehat{v}} \widehat{f}_\alpha \right) \right] + \right.$$
$$\left. \partial_x \left(v_{th,\alpha}^2 \widehat{v}_{||} \widehat{f}_\alpha \right) - v_{th,\alpha} \partial_x v_{th,\alpha} \left[\widehat{v}_{||} \widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\boxed{\underline{\underline{\Upsilon}}_{x,\alpha}} \vec{\widehat{v}} \widehat{v}_{||} \widehat{f}_\alpha \right) \right] \right\} = 0$$

- **Conservation of energy:**

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha \right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \gamma_{t,\alpha} \frac{\widehat{\nabla}_v}{2} \cdot \left(\vec{\widehat{v}} \widehat{f}_\alpha \right) \right] + \partial_x \left(v_{th,\alpha}^3 \widehat{v}_{||} \widehat{f}_\alpha \right)$$
$$- v_{th,\alpha} \partial_x v_{th,\alpha}^2 \left[\widehat{v}_{||} \widehat{f}_\alpha + \boxed{\gamma_{x,\alpha}} \frac{\widehat{\nabla}_v}{2} \cdot \left(\vec{\widehat{v}} \widehat{v}_{||} \widehat{f}_\alpha \right) \right] = 0$$

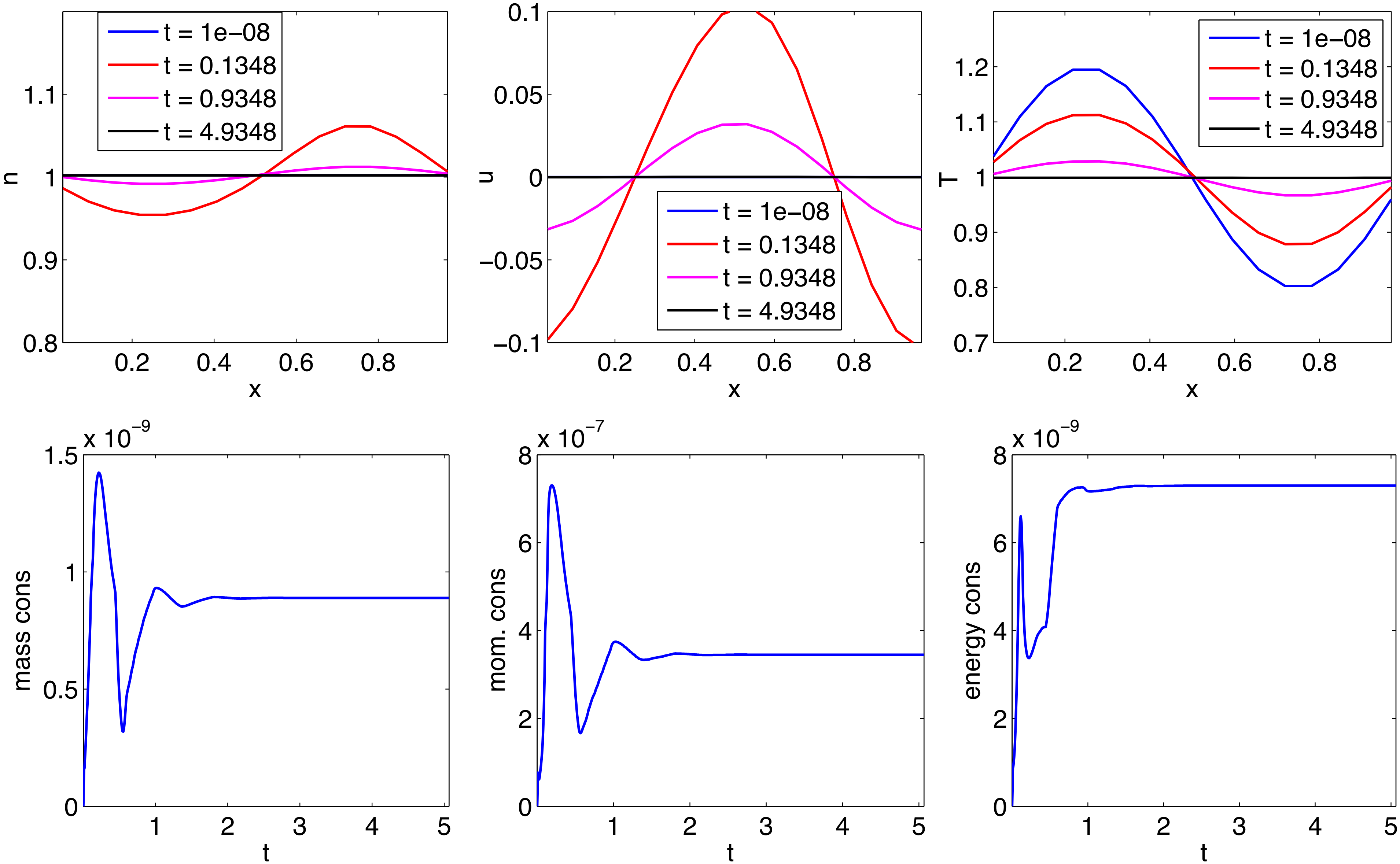
VE adaptivity in velocity space: All conservation laws

$$\partial_t \left(v_{th,\alpha}^2 \widehat{f}_\alpha\right) - \partial_t v_{th,\alpha}^2 \left[\widehat{f}_\alpha + \gamma_{t,\alpha} \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\vec{v}} \widehat{f}_\alpha\right)\right] + \partial_x \left(v_{th,\alpha}^3 \widehat{v}_{||} \widehat{f}_\alpha\right)$$
$$- v_{th,\alpha} \partial_x v_{th,\alpha}^2 \left[\widehat{v}_{||} \widehat{f}_\alpha + \gamma_{x,\alpha} \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\vec{v}} \widehat{v}_{||} \widehat{f}_\alpha\right)\right] + \xi_{t,\alpha} + \xi_{x,\alpha} = 0$$

Truncation error

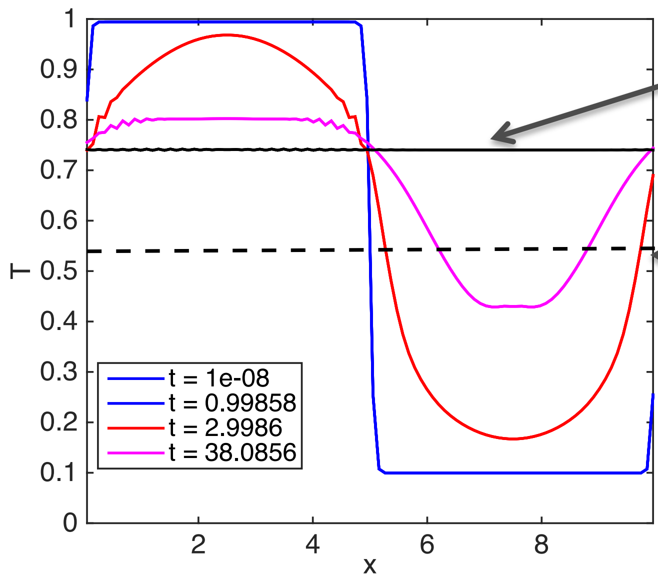
$$\xi_{x,\alpha} = v_{th,\alpha} \left\{\partial_x \left(v_{th,\alpha}^2 \widehat{v}_{||} \widehat{f}_\alpha\right) - v_{th,\alpha} \partial_x v_{th,\alpha} \left[\widehat{v}_{||} \widehat{f}_\alpha + \widehat{\nabla}_v \cdot \left(\underline{\underline{\Upsilon}}_{x,\alpha} \widehat{\vec{v}} \widehat{v}_{||} \widehat{f}_\alpha\right)\right]\right\} + \eta_{x,\alpha}$$
$$- \left\{\partial_x \left(v_{th,\alpha}^3 \widehat{v}_{||} \widehat{f}_\alpha\right) - v_{th,\alpha} \partial_x v_{th,\alpha} \left[\widehat{v}_{||} \widehat{f}_\alpha + \frac{\widehat{\nabla}_v}{2} \cdot \left(\widehat{\vec{v}} \widehat{v}_{||} \widehat{f}_\alpha\right)\right]\right\}$$

Relaxation of sinusoidal profile



Sharp profile relaxation problem: $T_{max}/T_{min} = 10$

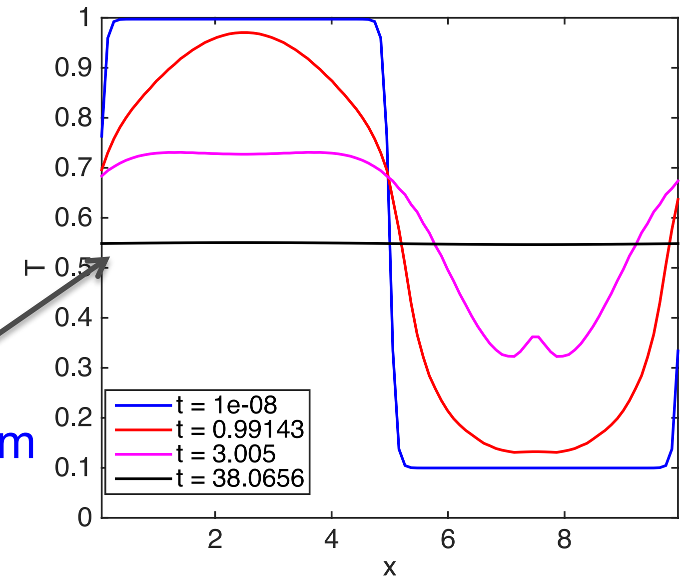
Non-conservative



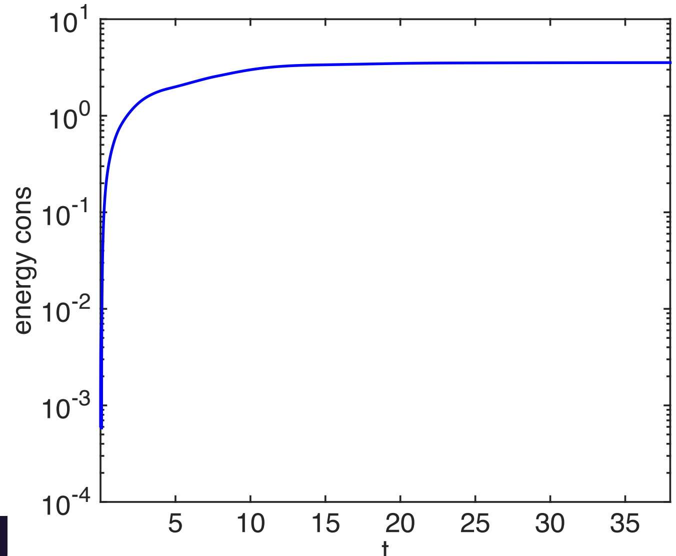
Wrong equilibrium due to numerical heating

Analytical equilibrium

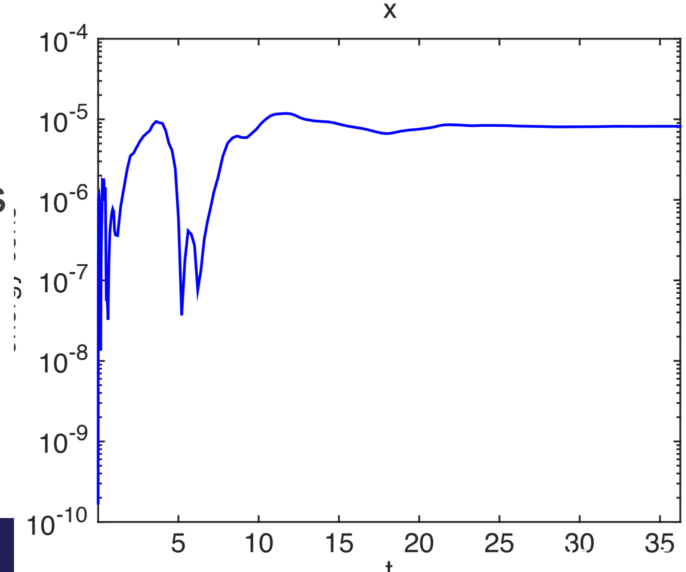
Conservative



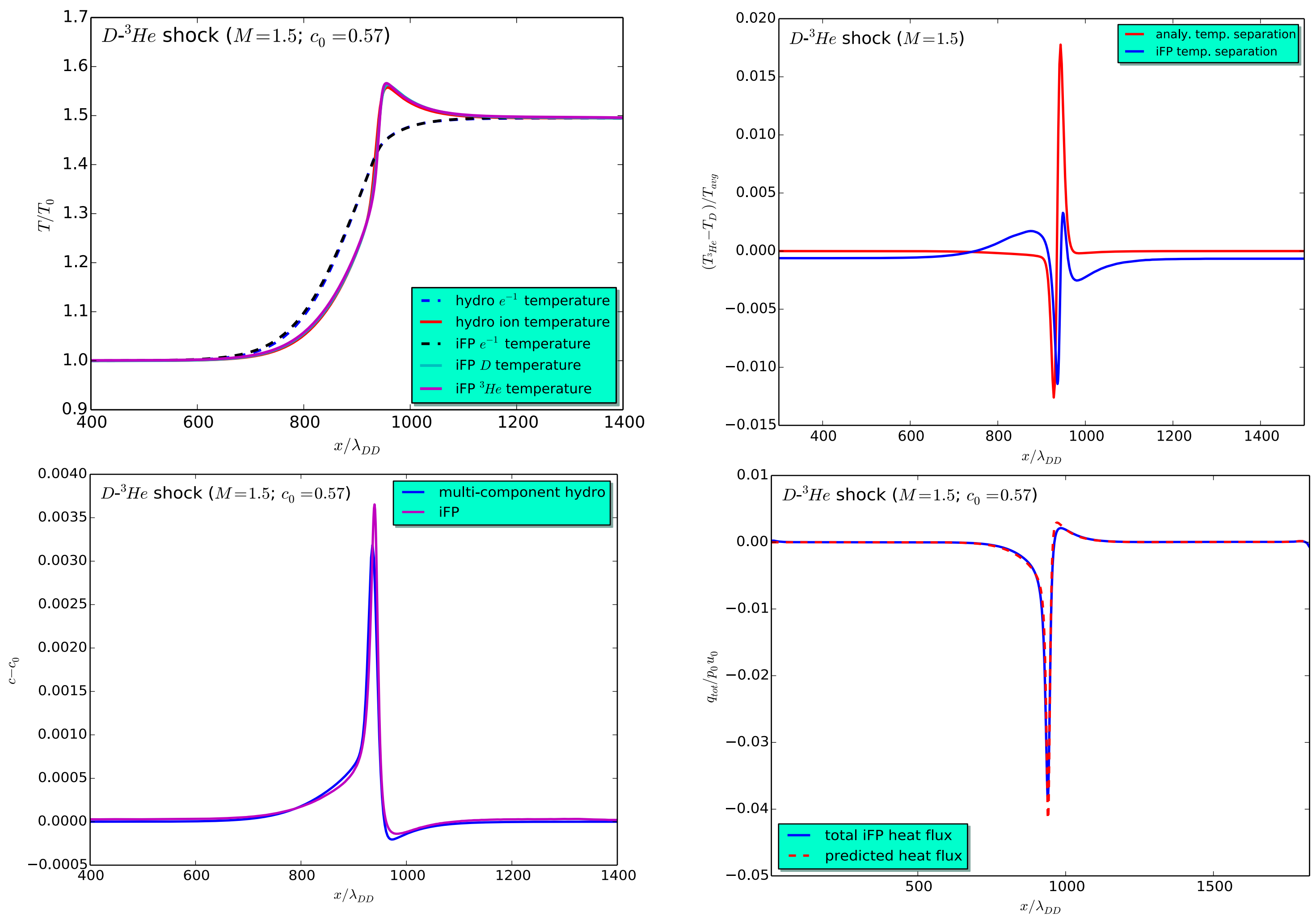
Correct equilibrium achieved



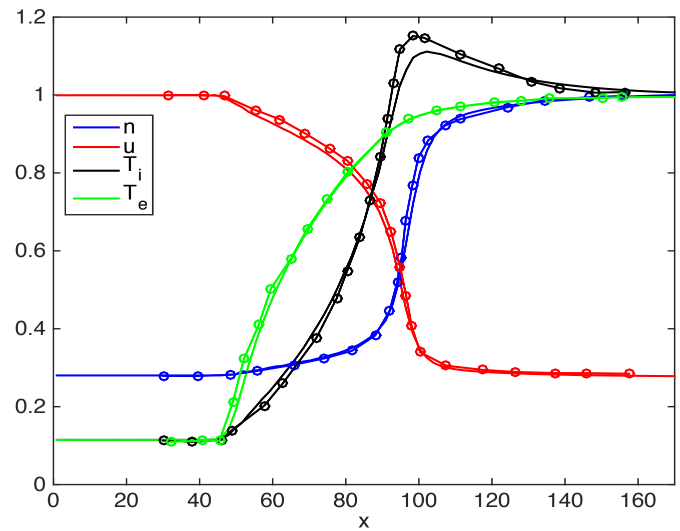
Velocity adaptation results in mesh savings of 10

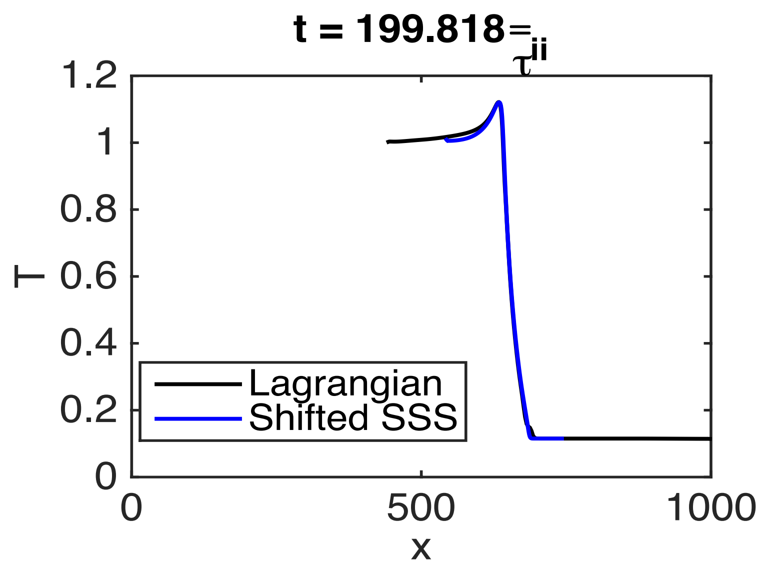


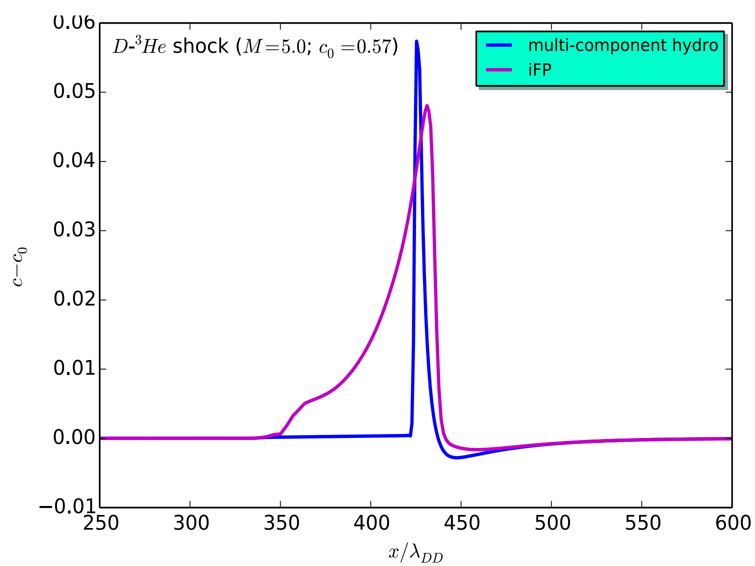
M=1.5 Shock (fluid regime)

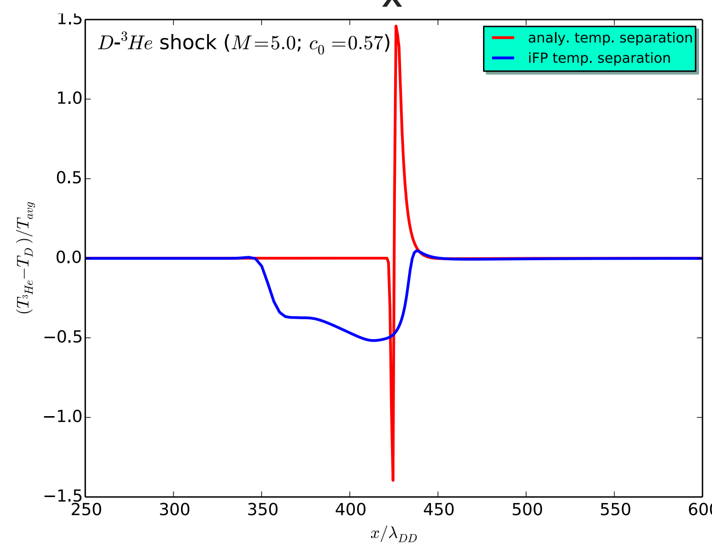


M=5 Shock (kinetic regime)

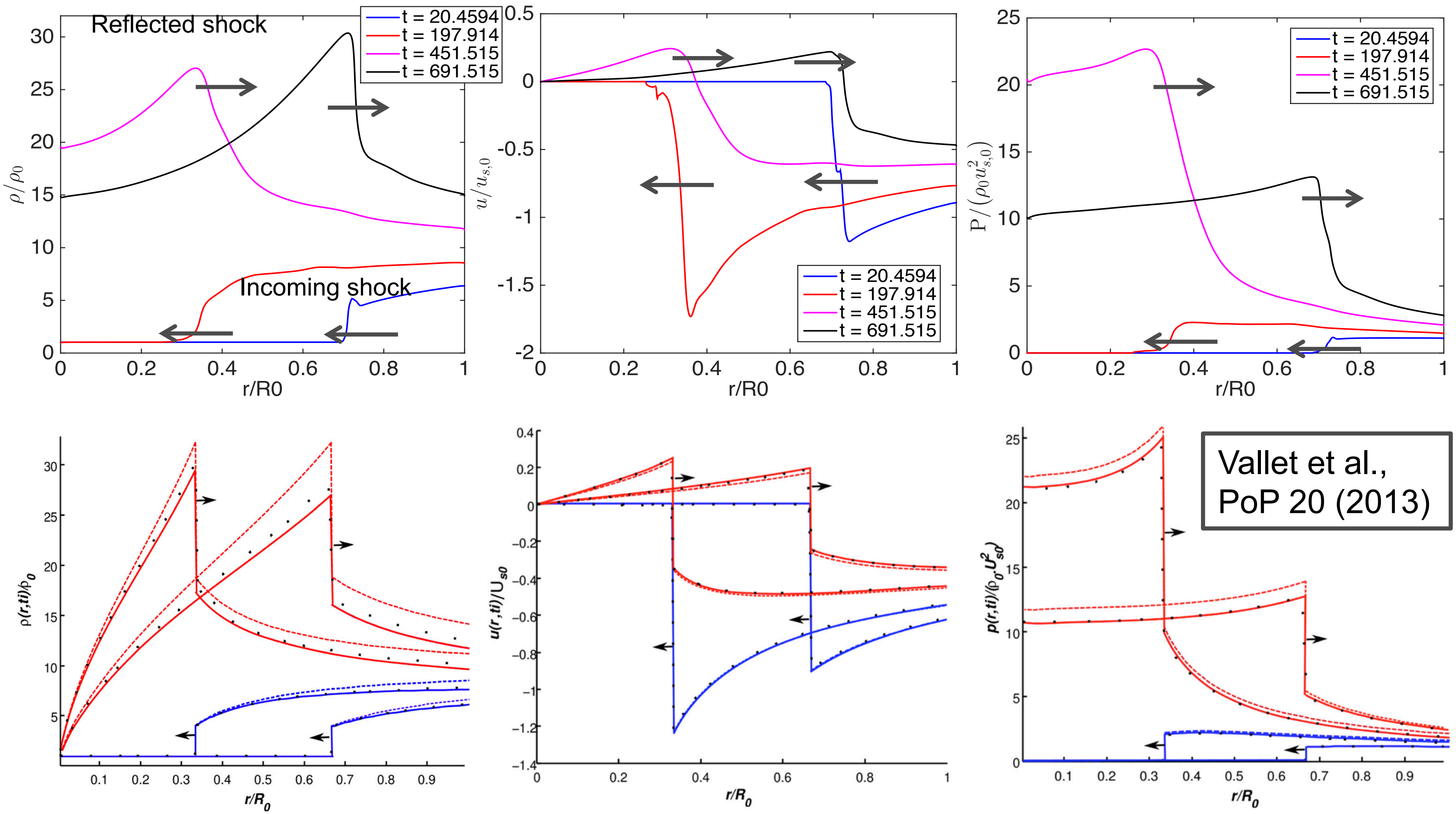








Guderley problem (M=10 shock in spherical geometry)

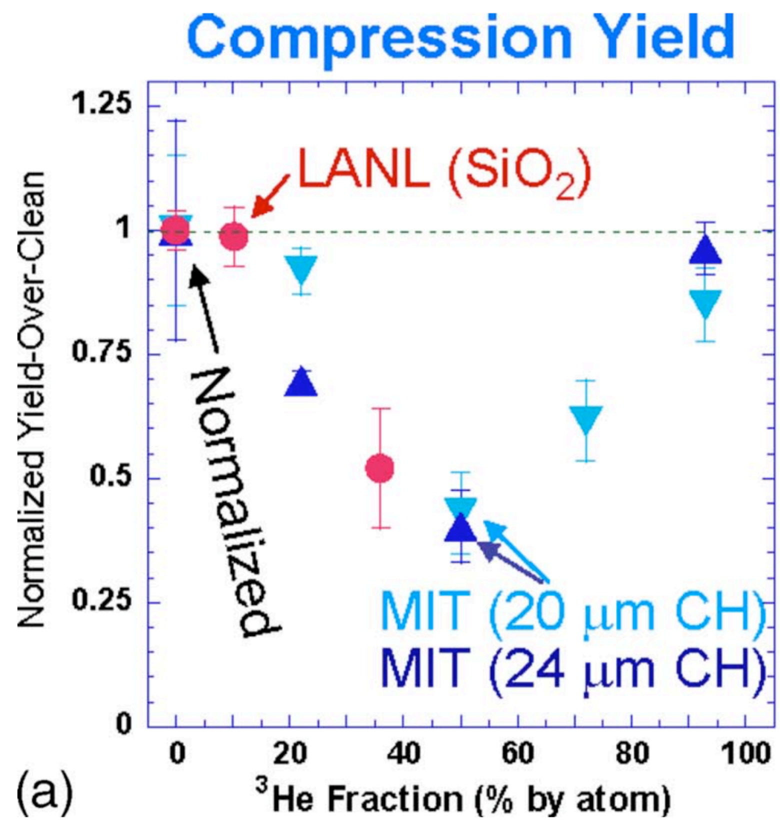


Application:

Species segregation effects on reactivity in ICF capsules (Rygg effect)

Rygg effect: An anomalous degradation in yield, relative to hydro simulation with varying conc.

- **Rygg et al. [PoP 2006] observed anomalous yield degradations relative to 1D clean hydro simulation for hydro-equivalent setups and varying concentration of species with charge to mass ratio i.e. Rygg effect**
- **A separate study by Hermann et al. [PoP 2009] confirmed these observations with different fuel composition**
- **Possibly attributed to species segregation and/or mix at pusher-fuel interface, compressibility reduction, etc.**



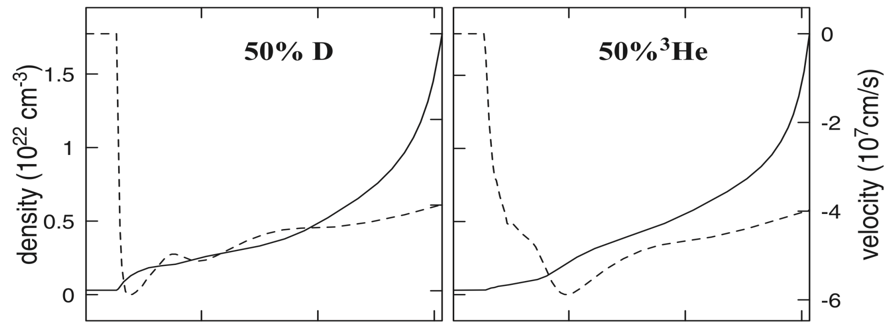
[Hermann et al. PoP 2009]

Kinetic simulation by FPION didn't see the Rygg effect

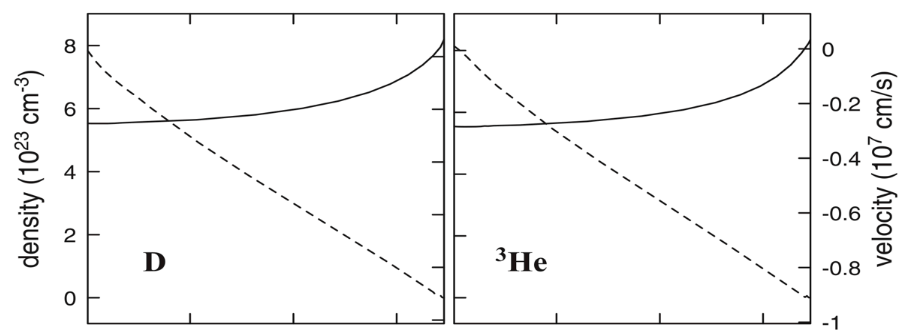
- 15 atm fill 50:50 D-He^3 Omega capsule simulation with hydro boundary for fuel [Larroche, PoP, 2012]

- **Species stratifies early on (shock convergence) but de-stratifies at compression**

- Slight yield degradation at shock bang, but not a factor of 2 seen by Rygg and Hermann



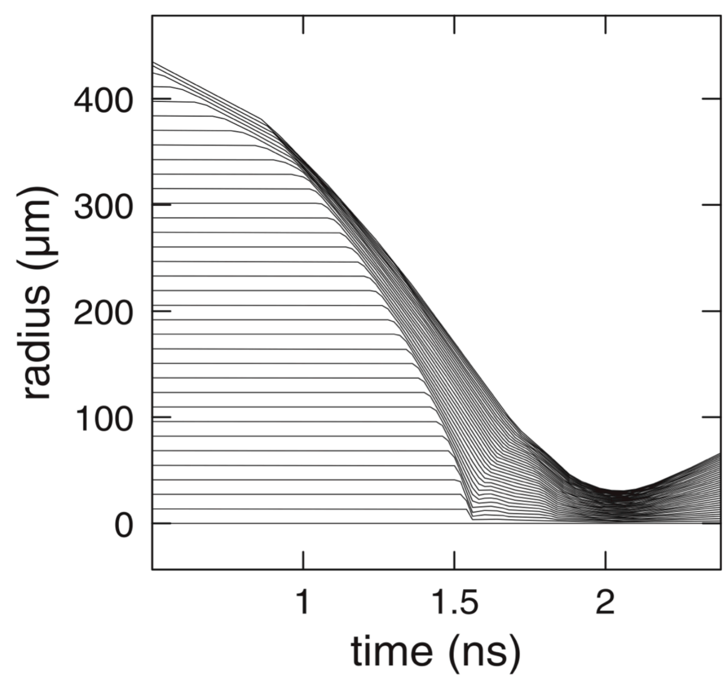
FPION: Density of D (left) and He3 (right) before shock convergence [Larroche, PoP 2012]



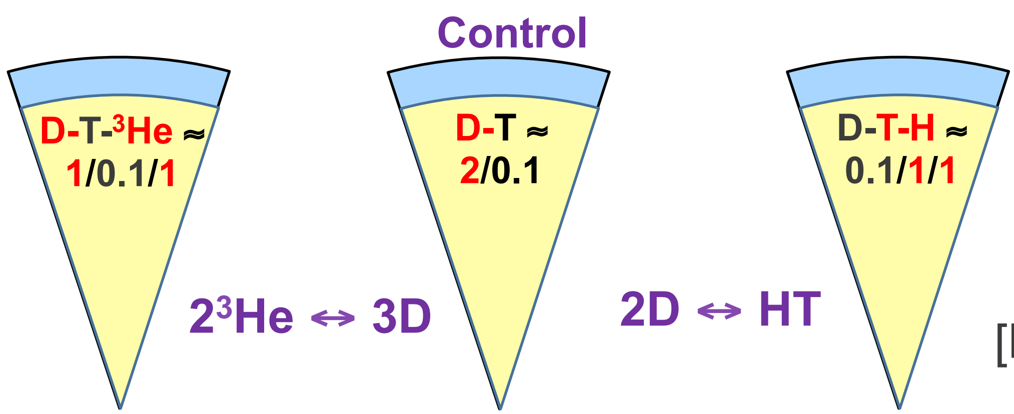
FPION: Density of D (left) and He3 (right) at compression [Larroche, PoP 2012]

A fuel-only kinetic simulation with hydro-equivalence

- **15 atm D-^{3}He fill Omega capsule simulation with hydro boundary at fuel/pusher interface [Larroche, PoP 2012, collaborator]**
- **We ignore ablator (pusher)**
- **We vary fuel concentration will ensuring hydro equivalence:**
  - **Same total mass density**
  - **Same total pressure (ion+electron)**

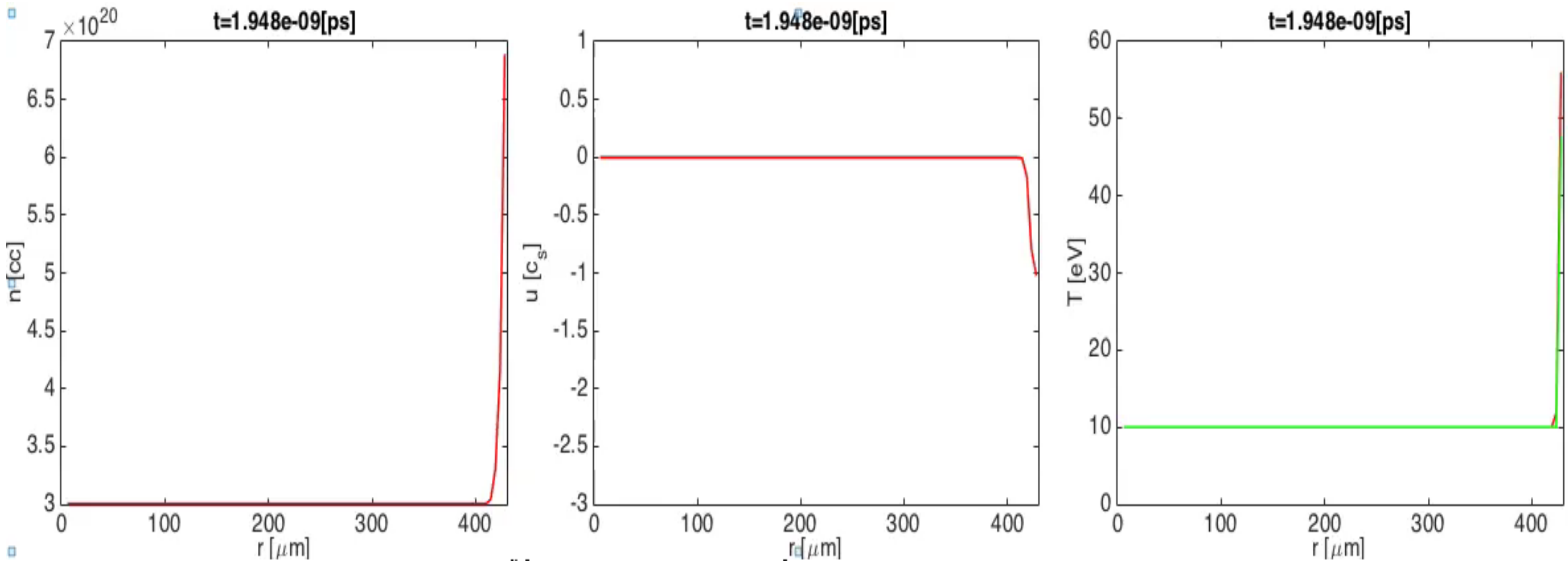


[Larroche, PoP 2012]

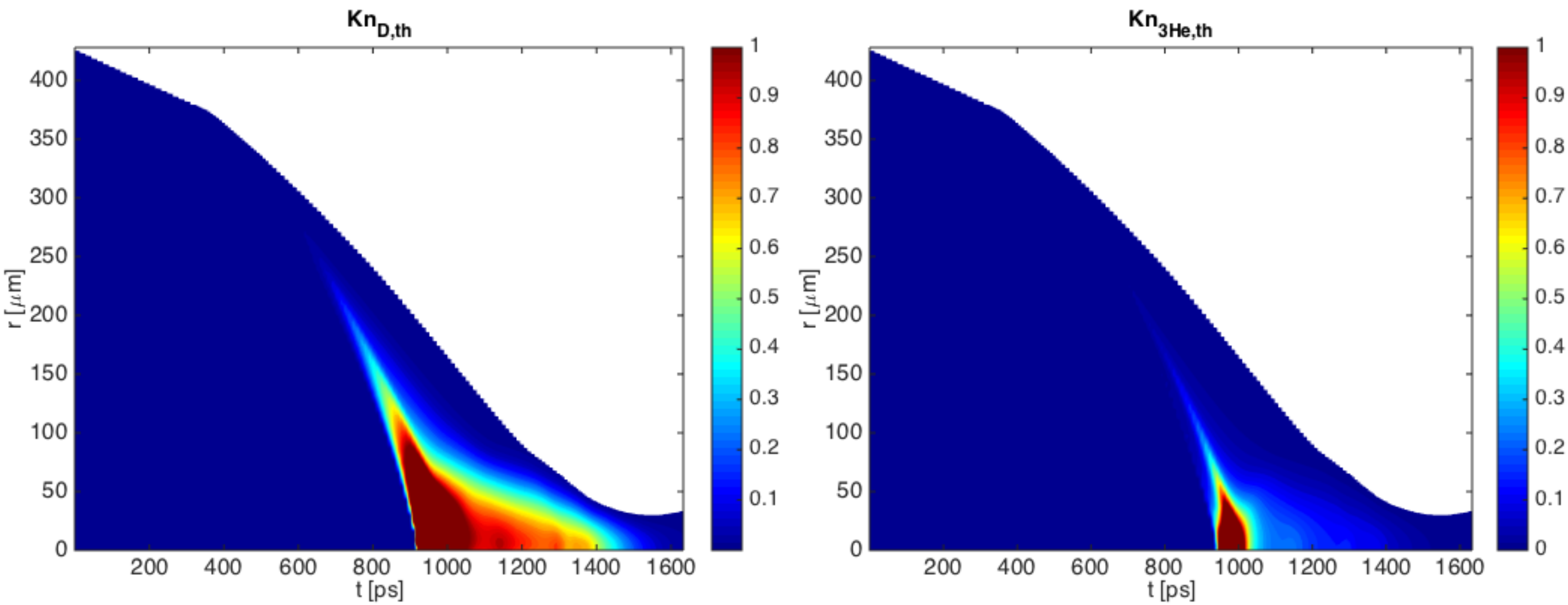


[Hermann et al., JOWOG37 2016]

iFP observes stratification surviving at later time

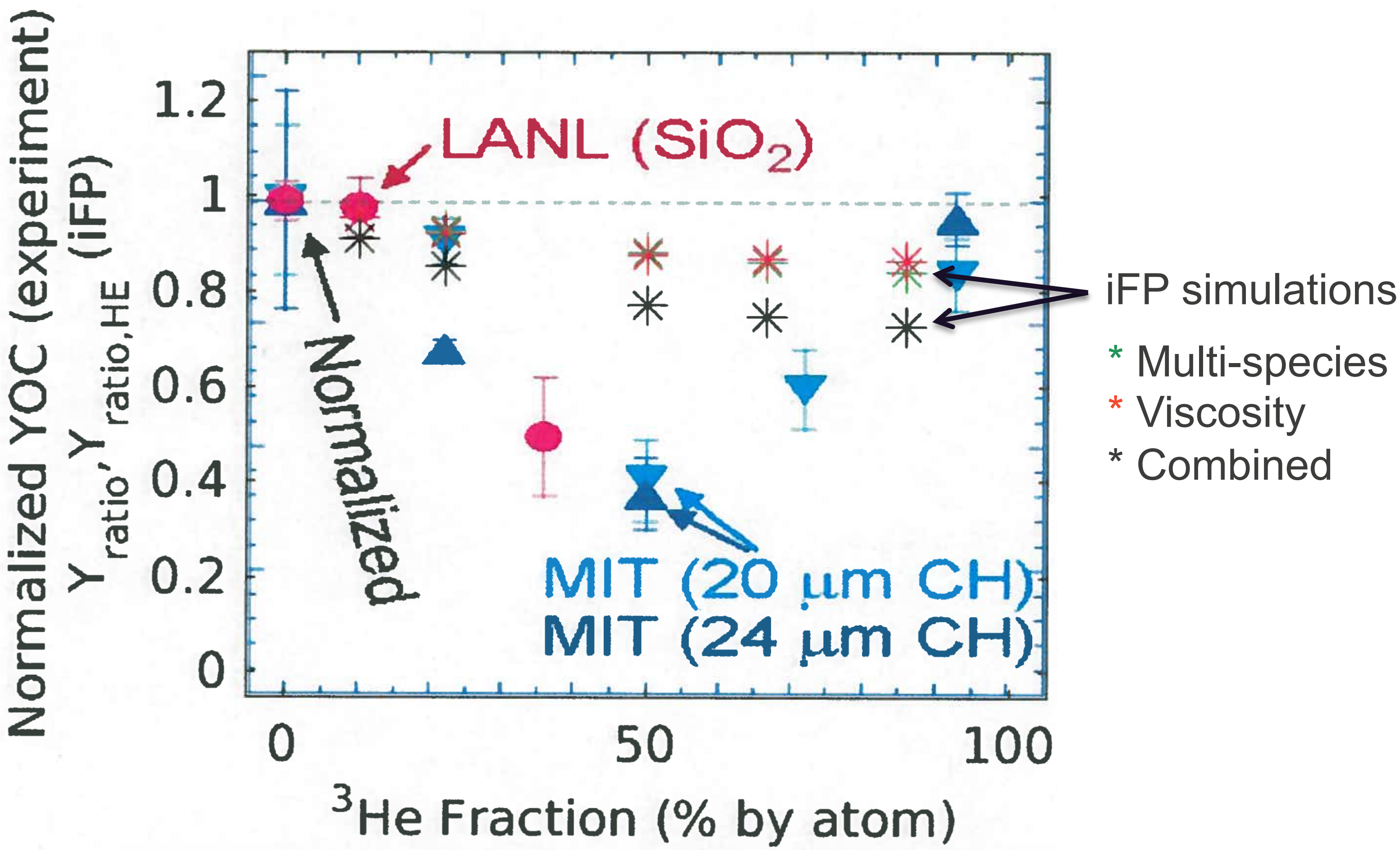


Kn reveals that D mean free path is on order capsule size for an appreciable time post shock convergence



$$Kn = \frac{\lambda_{mfp}}{R_{capsule}}$$

iFP matches yield trends in experiments



[Hermann et al. PoP 2009]

Conclusions

- **iFP is a first of a kind multi-scale simulation capability for ICF**
  - Implicit, scalable, adaptive, equilibrium preserving, strictly conserving
  - Strict verification campaign against hydro limit and other kinetic codes
- **iFP multiscale formulation and algorithm has transformed an intractable problem (beyond exascale) into a very approachable one (terascale)**
- **Algorithmic approach to Vlasov-Fokker-Planck equation has addressed long-standing issues in the field**
- **Began physics simulation campaigns**
  - For the first time, we have confirmed the impact of species segregation and plasma viscosity in reactivity
    - We did not find full agreement with experiments. Future work will include ablator.
  - Addressed controversies in literature on features of kinetic shocks (not discussed)